CHEMICAL PROCESS ANALYSIS AND OPTIMIZATION USING AN ANALOG COMPUTER

by 544

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PART I

ANALYSIS AND OPTIMIZATION OF AN AUTOCATALYTIC REACTION

Chapter 1

INTRODUCTION TO THE ANALOG COMPUTER

1. COMPUTER HISTORY AND CHARACTERISTICS (1, 2)

A computer is a device that is able to receive information (equations, instructions, data, etc.) and process it in a predetermined manner to obtain useable results. The history of computing devices may well extend to the very beginning of civilization. Computing devices can be divided into two categories: (1) mathematical instruments, the more complex of which are known as analog computers, and (2) calculating machines, more often known as digital computers. Early forms of digital computations could be considered to exist when man first started to use his fingers or pebbles for counting. The earliest known record of analog computation is its use in surveying and map making for the purpose of taxation (Babylonia, 3800 BC). The earliest digital machine is probably the abacus. In its early form, it consisted of a clay board with grooves in which pebbles were placed. The development of computational aids can be traced from these early instruments through the invention of logarithms, slide rules, linkages, analytical engines, and desk calculators to the large-scale general-purpose machines of the present day.

In digital computers, numbers are operated upon directly. The basic operation in these machines is counting. This enables the machine to perform the four fundamental operations of arithmetic, addition, subtraction, multiplication and division.

In analog machines, numbers are represented by physical quantities whose magnitudes are determined by the magnitudes of the numbers. Mathematical operations are represented by physical events; that is, the machines do not count, but perform continuous manipulations equivalent to the mathematical operation required.

2. COMPUTER SIMULATION (4)

Before one can apply automatic process control to individual plant units, one must know the dynamics or transient behavior of these plant units as well as their responses to various types of upsets, in the system. This information can be obtained in either of two ways. The first is through experiments on actual plant type equipment. The second is through "simulation" of the response of the actual equipment by mathematical means. Hence, one must derive the performance equations such that they represent the actual system as closely as possible.

In the case of analog computer simulation, the dependent variable being observed is the voltage at the output of any one of the several computing elements involved. Hence, any variation of these voltages represents directly the corresponding variations in the dependent variable of the actual system under study.

In addition, one can impose voltages onto the input of the computing elements of the computer which will represent any desired external influence on our actual physical system. Frequency responses of the actual system are also found by simulation since sinusoidal inputs can be applied to the computer. Thus a complete study of a particular chemical system can be made provided only that the assumptions upon which the simulation is based are accurate.

Process simulation will show the effect of external disturbances on control functions, the effect of environmental factors on process yields, product quality, and other vital points concerning the process. Thus the computer can help specify those operating conditions which will give a maximum return from the process.

3. THE ANALOG COMPUTER AND ITS BASIC PARTS (2, 5)

The general-purpose analog computer can perform specific mathematical operations and these, therefore, when connected together, can solve mathematical equations. The equations most suitable for solution on the computer are differential equations which contain only one independent variable, which is represented by time in the machine. Algebraic and partial differential equations can also be solved on the analog computer, but specific techniques are required and difficulties may arise in certain cases.

Analog computer components, each of which performs a specific mathematical operation, are classified either as linear or nonlinear components. The linear components perform the mathematical operations of

(a) multiplication by a constant

(b) inversion (change of sign)

(c) algebraic summation

(d) continuous integration.

These operations are sufficient to solve linear differential equations with constant coefficients.

The mathematical operations performed by nonlinear components are

(a) multiplication and division of variables

(b) the generation of arbitrary functions

(c) the mechanization of constraints and elementary logic operations.

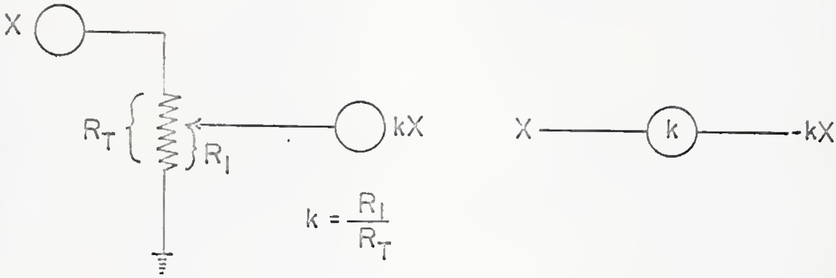
These components, together with the linear components, permit the analog computer to simulate the complex nonlinear systems which occur in practice.

A. Linear Components:

a. Attenuators

Multiplication of a d-c voltage by a positive constant which is less than unity is accomplished by a potentiometer (also called a "pot" or an attenuator). This device, shown in Figure 1, is simply a fixed resistor with a movable wiper arm. Two types of pots, "grounded" and "ungrounded" are used in the EAI TR-48 computer, of which 80% are grounded.

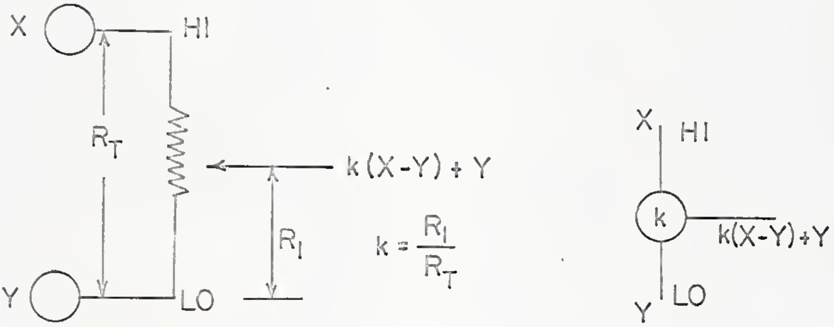
b. Operational Amplifiers



schematic diagram

symbollic diagram

(a) Grounded pot



schematic diagram

symbolic diagram

(b) Ungrounded pot

Fig. 1. Potentiometers or attenuators.

The operational amplifier is the basic unit in the analog computer. It can be used in a "summing mode" to perform any or all of the three linear operations of inversion, summation, and multiplication by a constant. It can also be used in an "integrating" mode" to integrate a voltage as the sum of a number of voltages with respect to time.

1. Inversion and multiplication by a constant

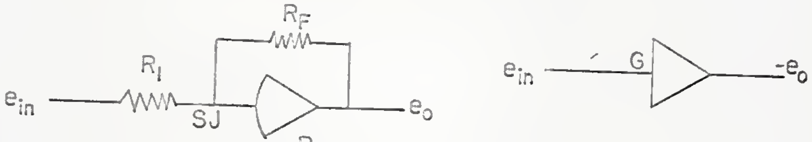
It can be shown that the output voltage of an amplifier is related to the input voltage as follows (5)

$$e_o = -\frac{R_F}{R_I} e_{in} \qquad (1)$$

From this equation it can be seen that the input-output relationship is solely dependent on the ratio of the feedback to the input resistances. In Figure 2(a), when both resistors are of equal magnitude, R, the amplifier output voltage has the same amplitude as the input voltage but is of the opposite polarity. Thus, the mathematical operation of inversion is performed:

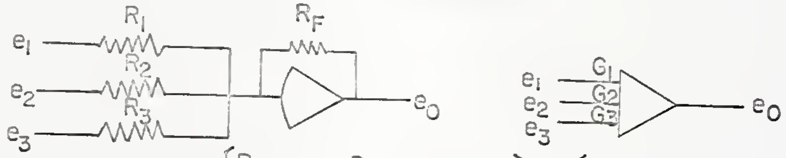
$$e_o = -\frac{R_F}{R_I} e_{in} = -\frac{R}{R} e_{in} = -e_{in} \qquad (2)$$

If the resistors are not of equal magnitude, the result is multiplication of the input by a constant, as shown in Figure 2(a).



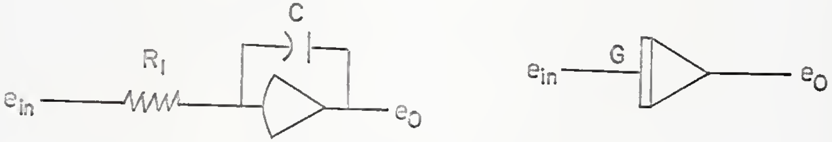
$$e_o = -\frac{R_F}{R_1} e_{in} = -G e_{in}$$

(a). Inversion and multiplication by a constant



$$e_o = -\left[\frac{R_F}{R_1} e_1 + \frac{R_F}{R_2} e_2 + \frac{R_F}{R_3} e_3\right] = -\left[G_1 e_1 + G_2 e_2 + G_3 e_3\right]$$

(b). Summation



$$e_o = -\frac{1}{R_1 C}\int_0^t e_{in}\,dt = G\int_0^t e_{in}\,dt$$

(c). Integration

Fig. 2. Schematic diagram and computer symbols for amplifier.

2. Summation

The addition of three parallel input resistors to the inversion circuit yields the summation as shown in Fig. 2(b).

$$e_o = - \left[\frac{R_F}{R_1} e_1 + \frac{R_F}{R_2} e_2 + \frac{R_F}{R_3} e_3\right] \qquad (3)$$

3. Integration

When the feedback resistor used in inversion circuits is replaced by a capacitor, the amplifier circuit becomes a simple integration circuit as shown in Fig. 2(c). It can be shown that (5)

$$e_o = \frac{1}{R_I C} \int_o^t e_{in} \, dt \qquad (4)$$

with no initial charge on the capacitor.

For multiple resistor inputs, the amplifier output voltage is the integral of the algebraic sum of the input voltages, that is,

$$e_o = - \int_o^t \left[\frac{e_1}{R_1 C} + \frac{e_2}{R_2 C} + . . . + \frac{e_N}{R_N C}\right] dt \qquad (5)$$

4. The Amplifier as a function generator

A method of generating an analytic function is to obtain a differential equation whose solution is the desired function. This equation can then be mechanized on the computer, with the proper initial conditions, to obtain the desired function. Typical examples are exponential and sinusoidal functions which are shown in Figures 3 and 4 respectively.

B. Non-linear Components (3, 5)

(a) Multipliers

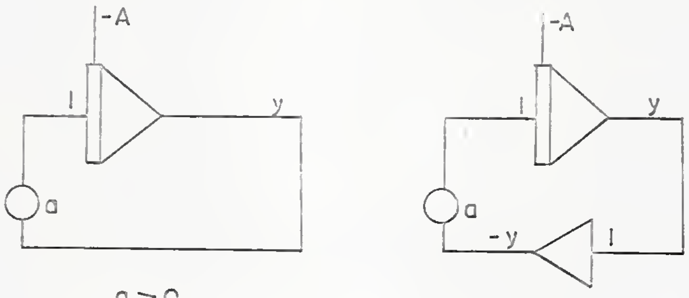
As the name suggests, a multiplier is a device which gives the instantaneous product of two time-varying voltages. The TR-48 analog computer has a quarter-square multiplier. This multiplier is based on the following identity:

$$xy = \frac{[(x+y)^2 - (x-y)^2]}{4} \tag{6}$$

This uses the current device with a high-grain amplifier to produce the multiplication. The current device is called a quarter-square card, which is shown in Figure 5(a).

(b) Function Generator

In many problems a variable y may be a function of another variable x. Furthermore, the functional relationship may be known analytically or graphically. The function generator is a device which relates two voltages according to a particular function relationship. A convenient symbol for function generator is shown in Figure



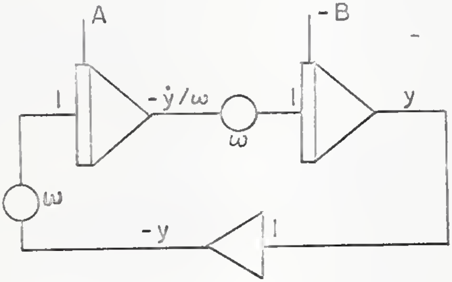
a > 0 a < 0

$$y = Ae^{-at}$$

$$\dot{y} = -aAe^{-at} = -ay$$

$$\therefore \; \dot{y} + ay = 0 \quad \text{and} \quad y(0) = A$$

Fig. 3. Exponential function using amplifer.



$$y = A\sin\omega t + B\cos\omega t$$

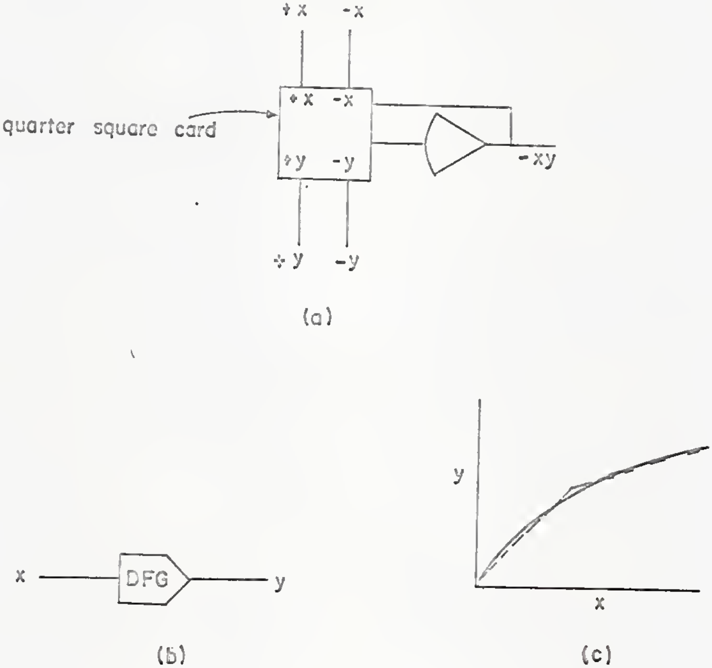
$$\dot{y} = \omega\left[A\cos\omega t - B\sin\omega t\right]$$

$$\ddot{y} = -\omega^2\left[A\sin\omega t + B\cos\omega t\right]$$

$$\therefore\ \ddot{y} + \omega^2 y = 0$$

$$y(0) = B \quad , \quad \dot{y}(0) = \omega A$$

Fig. 4. Sinusoidal function using amplifier.



(a)

(b)

(c)

Fig. 5. (a). Quarter-square multiplier.

(b). Function generator.

(c). y = f(x) from function generator.

5(b). The most common function generator now used is the diode function generator. This device actually approximates a function y = f(x) by a number of straight-line segments which are joined together as illustrated in Figure 5(c).

C. Analog Memory

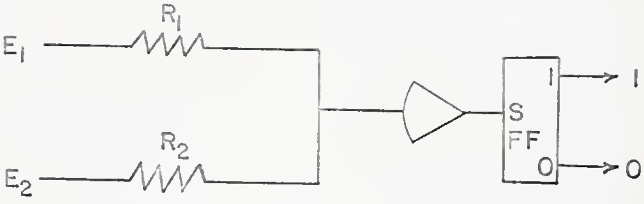
Memory, or storage ability of an analog computer (very restrictive compared to digital computers), can greatly increase its problem solving capacity. Typical classes of applications for storage techniques include the following (i) Automatic Iteration and (ii) Parameter sweep.

(a) Comparator Mode

Figure 6(a) shows the block diagram for the electronic comparator when it is in the comparator mode. The input signals are applied to resistors and are summed at a summing junction which is patched to an asynchronous flip-flop. When the sum of the inputs is positive, a negative signal from the amplifier sets the flip-flop with the "1" output at binary one and "0" output at binary zero, and vice versa when the input sum is negative.

(b) Simple Track and Store Unit

A program symbol for a track-store unit is shown in Figure 6(b). The logic input signal controls the switching between the track and store modes. The unit tracks when the logic input is binary one, and it holds when the logic input is binary zero. The binary inputs may be applied from the output of a comparator or from external digital equipment.



(a)

Note : (1). When $E_1 + E_2 \geq 1.0$ MV

1 Output = Binary 1

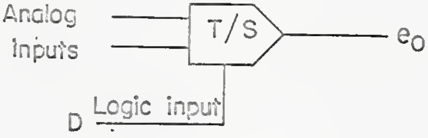
0 Output = Binary 0

(2). When $E_1 + E_2 \leq 1.0$ MV

1 Output = Binary 0

0 Output = Binary 1

(a). Electronic comparator mode



(b)

Note : (1). When D is binary 1 , amplifier tracks

(2). When D is binary 0 , amplifier stores

(b). Electronic track and store modes

Fig. 6 . Electronic comparator mode and Electronic track and store modes.

4. RECORDING EQUIPMENT (3, 5)

A computer solution to a problem is in the form of a time-varying voltage signal, and instruments are needed to indicate and record this voltage-time relationship. A simple indicating device is a voltmeter. If a record is wanted, a strip-chart recorder or xy recorder can be used.

An xy recorder is a two-axis graphic voltage recorder which provides a flat-bed recording surface that holds a sheet of ordinary graph paper. Recording is accomplished by a pen supported in a dual-axis carriage.

Another popular recorder in analog computation is the common two-channel oscilloscope; in this case, the signal is traced by a spot of light generated by an electron beam moving across the face of the cathode-ray tube. The oscilloscope is used to record signals by a method called repetitive operation in which the solution is repeated over and over at a rapid rate, with the result that the spot of light following the signal leaves a continuous visible trace on the screen of the oscilloscope. The solution is repeated at a rate which may vary from 10 to 100 or 500 times faster per second. The computer contains a special time-sequencing device which will automatically perform the operation of applying initial condition voltages, starting the solution and so on. Because of the rapid rate at which the solution is repeated, one can observe immediately the change in the shape of the solution curve as problem parameters are changed. For this reason repetitive operation is extremely useful in the study of the transient behavior of a system as parameters are varied.

5. SCALING

The computer voltage and solution time are analogous to the dependent and independent problem variables, respectively. Furthermore, when the computer is programmed directly from the problem equations, there is a one to one relationship between the computer and problem variables; that is, one volt corresponds to one unit of the problem dependent variable, and one unit of computer time corresponds to one unit of the problem independent variable. However, the computer has inherent limitations which bound the range of errorless operation of each of the components. To insure that the computer does not attempt to solve the problem outside the proper operating range, one must often modify the simple one-to-one scaling between the computer and problem variables.

Amplitude scaling changes the voltage level of the components; time scaling alters the length of time required by the computer to solve the problem. The constant relating the two is called the scale factor in each one.

$$\text{magnitude scale factor} = K = \frac{\text{Reference Voltage}}{\text{Maximum value of Problem variable}}$$

$$\text{time-scale factor} = \beta = \frac{\text{Computer time}}{\text{Problem time}} \tag{7}$$

All components other than the integrators of the analog computer are unaffected by time-scaling.

If $\beta > 1$, then the solution on the computer is slower than the original process; if $\beta < 1$, the computer solution is faster than the original process.

6. THE STATE VARIABLE APPROACH AND ANALOG SUBROUTINES (29)

a. Concept of the State Variable (3)

Consider the general nth-order ordinary differential equation, written in a form which is solved for the highest derivative

$$\frac{d^n x}{dt^n} = f\left(x, \frac{dx}{dt}, \frac{d^2 x}{dt^2}, \ldots, \frac{d^{n-1} x}{dt^{n-1}}\right) \qquad (8)$$

Suppose that the new variables $(x_1, x_2, \ldots, x_n)$ are defined by the following relations.

$$\begin{aligned} x_1 &= x \\ x_2 &= \frac{dx}{dt} \\ x_3 &= \frac{d^2 x}{dt^2} \\ &\ldots \\ x_n &= \frac{d^{n-1} x}{dt^{n-1}} \ . \end{aligned} \qquad (9)$$

In other words, the dependent variable of the nth-order differential equation is defined at the first state variable and the first order derivative as the second state variable and so on in an ascending order and finally the (n-1)th order derivative is defined as the nth state variable. Then, equation (9) may be rewritten as a system of n simultaneous first-order equations,

$$\begin{aligned} \frac{dx_1}{dt} &= x_2 \\ &\vdots \\ \frac{dx_{n-1}}{dt} &= x_n \\ \frac{dx_n}{dt} &= f(x_1, x_2, \ldots, x_n, t). \end{aligned} \tag{10}$$

This implies that an ordinary differential equation of any order can be considered as a set of first order ordinary differential equations. This system of equations, Equation (10), is called the state-space or phase-space representation of Equation (8). The variables (x_1, x_2, x_3, . . ., x_n) are called state variables and they are also the coordinates of the phase-space. The advantage of this representation lies in the fact that it represents linear and non-linear equations in a uniform manner. This representation of an ordinary differential equation is consistent with the way it is solved by analog computation. For example, each differential operation corresponds to a single integration. In general one can fairly easily see from this representation of equations that integrators, multipliers, etc. are needed for the problem.

b. Subroutines for Analog Computation (29)

There are many ways of drawing an analog computer diagram for solving an ordinary differential equation. But one can usually divide the analog diagram into three systematic subdiagrams or analog subroutines, namely, (1) the analog main subroutine, (2) the analog special function subroutine, and (3) the analog memory subroutine. The analog main subroutine may consist chiefly of the diagrams of unconnected components which perform integration, summation, sign inversion, and multiplication by a constant and multiplication by a variable. Analog special function subroutines consist of standard function generating circuits which can give rise to special functions such as the sine, cosine, hyperbolic sine, hyperbolic cosine, and exponential functions. It also contains function generator circuits which can mix any desired functions. An analog memory subroutine may contain a diagram for a comparator circuit, a track and store circuit, or a digital memory circuit. Figures 7 and 8 show the typical analog subroutines. Note that the main subroutine must be completed by the programmer, who must also supply the connections with other subroutines which may be on the separate sheets. Also some minor supplemental work is often needed to complete the special function subroutines to modify the functions

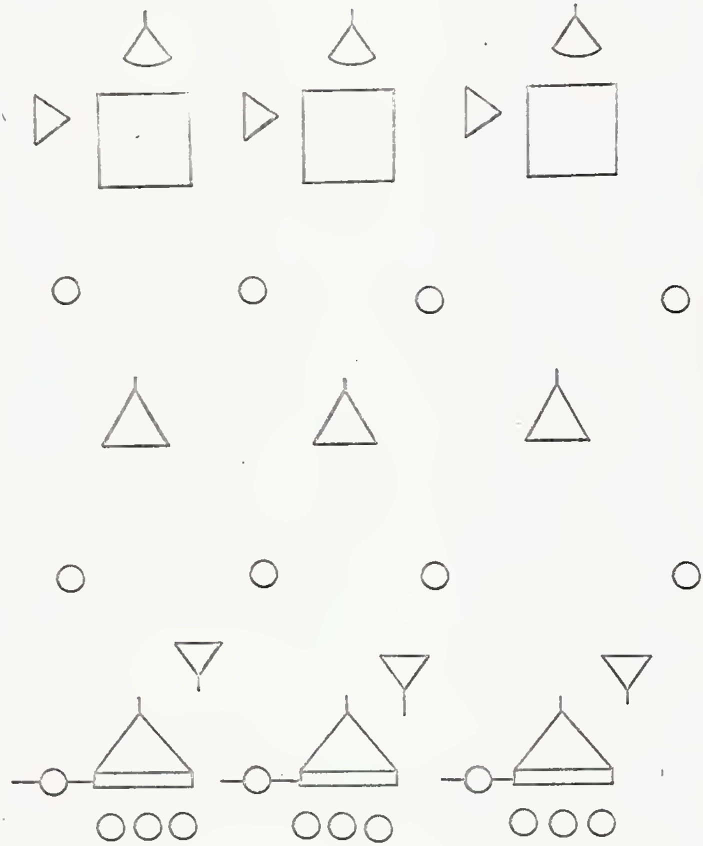
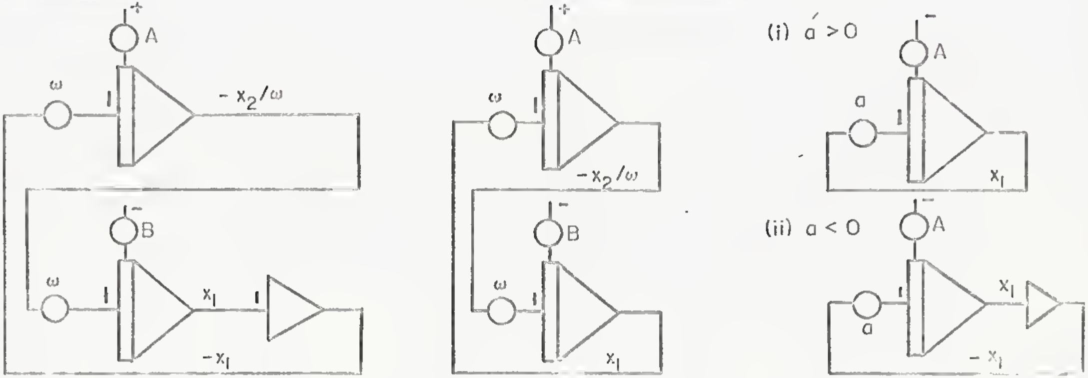


Fig. 7. Analog main subroutine.



$x_1 = A \sin\omega t + B \cos\omega t$

$$\frac{dx_1}{dt} = \omega\left[A \cos\omega t - B \sin\omega t\right]$$

$$= x_2$$

$$\frac{dx_2}{dt} = -\omega^2 x_1$$

$x_1(0) = B \quad , \quad x_2(0) = \omega A$

Sinusoidal Function

$x_1 = A \sinh\omega t + B \cosh\omega t$

$$\frac{dx_1}{dt} = \omega\left[A \cosh\omega t + B \sinh\omega t\right]$$

$$= x_2$$

$$\frac{dx_2}{dt} = \omega^2 x_1$$

$x_1(0) = B \quad , \quad x_2(0) = \omega A$

Hyperbolic Function

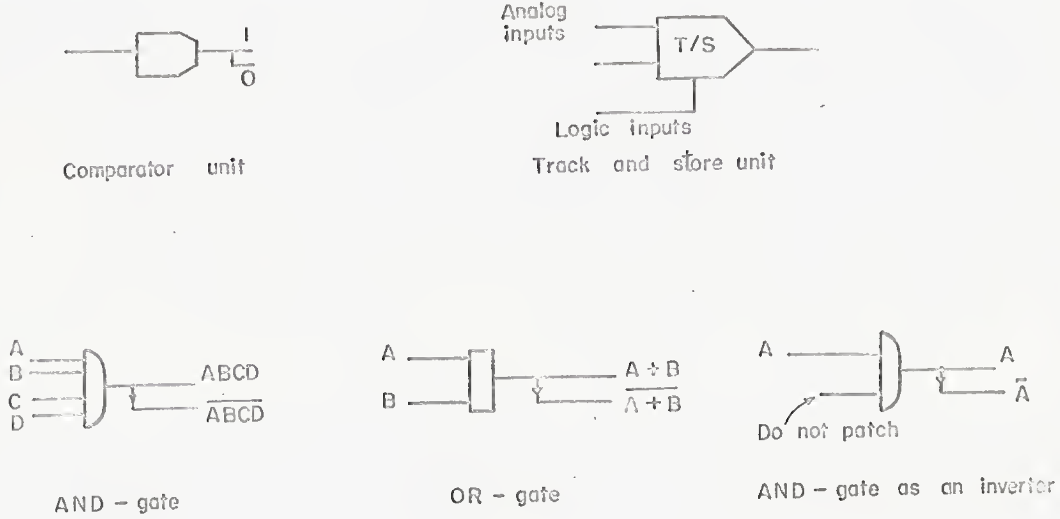
$x_1 = Ae^{-at}$

$$\frac{dx_1}{dt} = -ax_1$$

$x_1(0) = A$

Exponental Function

Fig. 8(a). Analog special functions subroutines.



Comparator unit

Track and store unit

AND - gate

OR - gate

AND - gate as an inverter

Fig. 8 (b). Comparator unit and analog - memory subroutines.

to suit individual problems. It is worth noting that these subroutines can be printed out beforehand for later uses. As an illustrative example, one may consider the problem of axial diffusion in an isothermal tubular flow reactor.

Material balances in a tubular flow reactor operated under isothermal steady state conditions yield the following equations:

$$\frac{d}{dz}\left(D_A \frac{dC_A}{dz}\right) - u \frac{dC_A}{dz} + r_A = 0 \tag{11}$$

and

$$\frac{d}{dz}\left(D_B \frac{dC_B}{dz}\right) - u \frac{dC_B}{dz} + r_B = 0 \tag{12}$$

where

D_i = axial dispersion coefficient of reactant i

C_i = concentration of reactant i

u = mean linear velocity of reacting mixture

r = rate of reaction

z = co-ordinate in the direction of flow.

Suppose that the following biological reactions are taking place in the reactor.

$$-r_A = \frac{k\ C_A\ C_B}{K + C_A}$$

and

$$r_B = \frac{k\ C_A\ C_B}{K + C_A} - k_D\ C_B$$

where k and k_D are rate constants and K is a system parameter. Substitution of the above two expressions into Equations (11) and (12) gives

$$\frac{d}{dz}\left(D_A \frac{dC_A}{dz}\right) - u \frac{dC_A}{dz} - \frac{k\ C_A\ C_B}{K + C_A} = 0 \qquad (13)$$

and

$$\frac{d}{dz}\left(D_B \frac{dC_B}{dz}\right) - u \frac{dC_B}{dz} + \frac{k\ C_A\ C_B}{K + C_A} - k_D\ C_B = 0 \qquad (14)$$

respectively. It is also assumed that the respective axial dispersion coefficients vary respectively according to the following relationships,

$$D_A = \alpha(1 + \beta\ \sin \omega z)$$

and

$$D_B = \gamma e^{\delta z} .$$

According to the state variable approach, let

$$x_1 = C_A$$

$$x_2 = D_A \frac{dC_A}{dz}$$

$$x_3 = C_B$$

$$x_4 = D_B \frac{dC_B}{dz}$$

This gives rise to the following four first order differential equations,

$$\frac{dx_1}{dz} = \frac{x_2}{\alpha(1 + \beta \sin \omega z)}$$

$$\frac{dx_2}{dz} = \frac{k\ x_1\ x_3}{K + x_1} + u\left[\frac{x_2}{\alpha(1 + \beta \sin \omega z)}\right]$$

$$\frac{dx_3}{dz} = u\ \frac{x_4}{\lambda e^{\delta z}}$$

$$\frac{dx_4}{dz} = -\ \frac{k\ x_1 x_3}{K + x_1} + k_D\ x_3 + u\ \frac{x_4}{\lambda e^{\delta z}}$$

Using the analog subroutine scheme described earlier, the computer diagram for the above system of equations is drawn as shown in Figure 9.

It can be seen that the state variable approach enables one to determine how many components are needed for analog computation. For example, one can see from the above four differential equations for four state variables that one needs four integrators, four multipliers and two special function generating circuits. One can see also that there is only one input into integrator one and also integrator three for the first and third differential equations. Similarly, there are two inputs for the second differential equation and three inputs for the fourth differential equation. Hence, there are seven inputs in all and thus one needs at least seven pots. One also needs four more pots for initial conditions on each of the integrators.

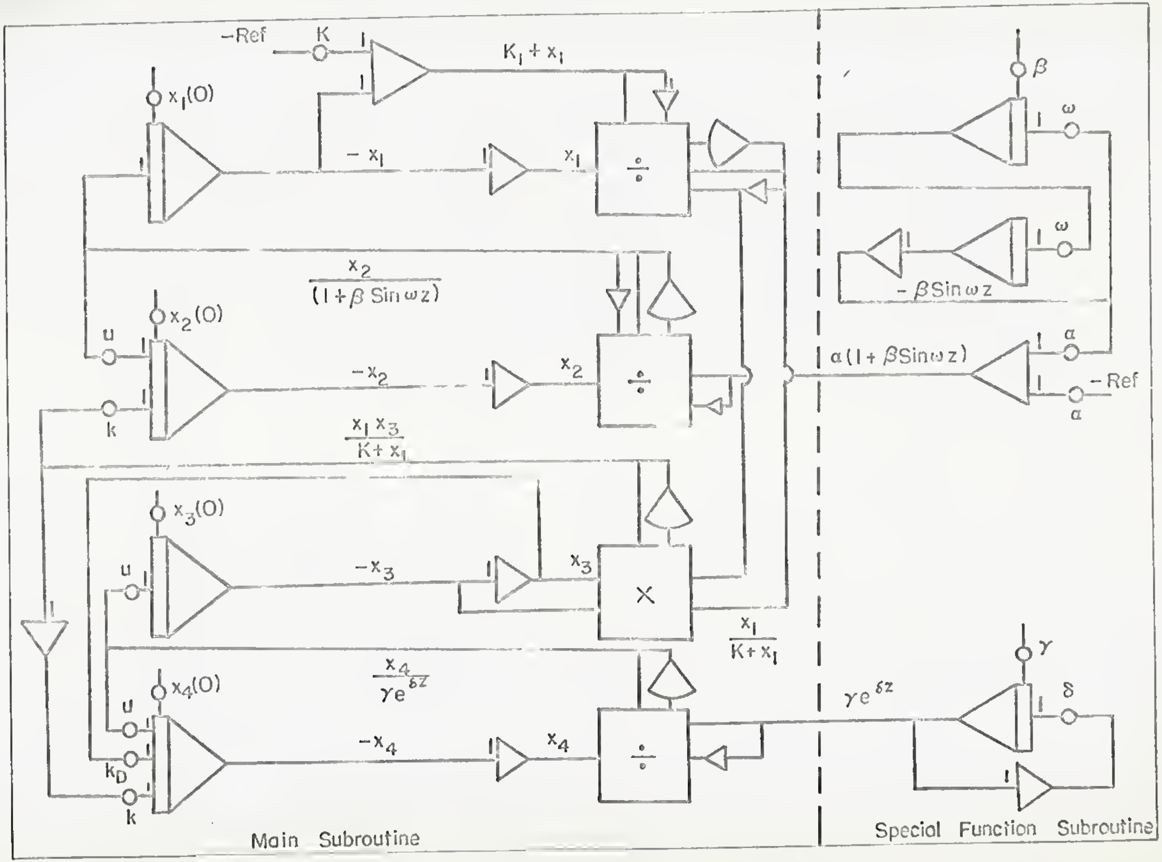


Fig. 9. Analog diagram for the axial diffusion reactor problem.

Chapter II

INTRODUCTION TO THE AUTOCATALYTIC REACTION PROBLEM

1. INTRODUCTION

A reaction in which one of the products of the reaction acts as a catalyst is called an autocatalytic reaction. Examples of autocatalytic reactions are found generally in the acid-catalyzed hydrolysis of various esters and similar compounds and in various biochemical processes such as waste treatment. The rate of reaction is influenced by the concentration of some of the products as well as that of some of the reactants. Therefore, the rate of an autocatalytic reaction in a continuous flow reactor is influenced by two important factors; these are the initial concentration of the autocatalytic agent and the temperature at which the reaction is carried out. It is assumed that there is a macromixing and micromixing within the continuous flow reactor.

Since in autocatalytic reactions the rates are influenced by both reactants and products, these reactions deserve special attention, which leads to optimization problems (10).

The purpose of part I of this report is to present a relatively simple optimization study of autocatalysis involving only two consecutive kinetic steps with rate constants k_1 and k_2.

$$A \xrightarrow{k_1} B \qquad \text{initiating reaction} \qquad (15)$$

and

$$A+B \xrightarrow{k_2} 2B \qquad \text{autocatalytic step} \qquad (16)$$

where k_1 is much smaller than k_2, and B is the desired product. The specific aim is to minimize the total residence time or the total mean holding time of the system for any desired conversion.

An isothermal system is considered, in which a continuous stirred tank reactor (CSTR) is followed by a plug flow tubular reactor (PFTR) as shown in Figure 10. Since the CSTR preceeds the PFTR, a small amount of B is formed by the first reaction [Equation 15] and completely mixed with the reactant in the CSTR. The resulting mixture is then fed into a PFTR to achieve as much conversion of B as possible. If a CSTR is not used in the upstream and instead only a PFTR is used, extra holding time or extra length of a PFTR will be required to promote appreciably the first reaction [Equation (15)].

The pure A is fed into a CSTR and it is assumed that the system is at its steady state and the molal feed rate F remains constant throughout the process. This optimization problem is solved on an analog computer (EAI model TR-48).

The general procedures for preparing kinetic problems for analysis by analog computer have been discussed by T. J. Williams (6).

2. KINETIC STEPS FOR SIMPLE AUTOCATALYSIS (7, 8)

Reactant A can decompose via two routes, a slow uncatalyzed one (k_1) and another catalyzed by B(k_2). The two essential kinetic steps are

$$A \xrightarrow{k_1} B \qquad \text{initiating reaction} \qquad (15)$$

$$A+B \xrightarrow{k_2} 2B \qquad \text{autocatalytic step} \qquad (16)$$

These equations show that the first reaction (k_1) is the starter, but continues concurrently with the second reaction (k_2) as long as there is any A left in the reacting stream. The second reaction (k_2) is the path by which most of A decomposes.

The rates of formation of A and B in accordance with the two kinetic steps shown above are

$$r_A = \frac{dC_A}{dt} = -k_1C_A - k_2C_AC_B \qquad (17)$$

and

$$r_B = \frac{dC_B}{dt} = k_1C_A - k_2C_AC_B + 2k_2C_AC_B$$

or

$$r'_B = \frac{dC_B}{dt} = k_1C_A + k_2C_AC_B \qquad (18)$$

where

C_A = concentration of A, moles/ft^3

C_B = concentration of B, moles/ft^3

If one defines x_A equal to the mole fraction of A, then

$$A \xrightarrow{k_1} B$$

$$A + B \xrightarrow{k_2} 2B$$

$$\text{where} \quad k_1 <<< k_2$$

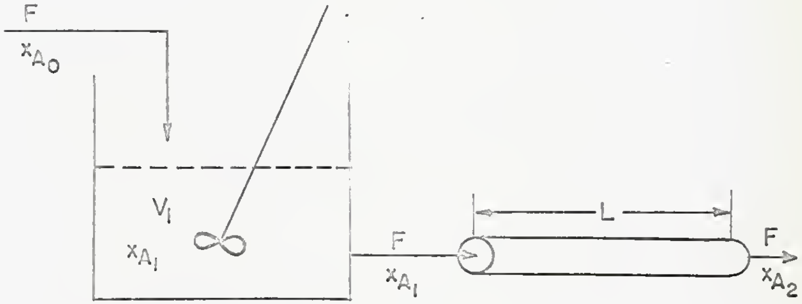


Fig. 10. Autocatalytic reaction taking place in a CSTR and followed by a PFTR.

$$x_A = \frac{C_A}{\rho} = \left(\frac{\text{moles of A}}{\text{ft}^3}\right)\left(\frac{\text{ft}^3}{\text{moles of mixture}}\right) \qquad (19)$$

where ρ is the density of the reactant and product mixture with the units of moles of mixture/ft^3. This will be assumed to remain constant throughout the reactor, and hence the rate of disappearance of A can be written from Equation (17) as

$$(-r_A) = -\frac{d(x_A\rho)}{dt} = +\,[k_1 x_A\rho + k_2 (x_A\rho)\ (x_B\rho)]$$

But x_B is the mole fraction of B and is equal to $(1-x_A)$. Therefore, one can write the above expression as

$$(-r_A) = -\frac{d(x_A\rho)}{dt} = +\,[k_1\rho x_A + k_2\rho^2 x_A\ (1-x_A)] \qquad (20)$$

where

$$r_A = \frac{\text{moles A}}{(\text{ft}^3)(\text{sec})}$$

or

$$(-R_A) = -\frac{dx_A}{dt} = +\,[k_1 x_A + k_2\rho x_A (1-x_a)] \qquad (21)$$

where

$$R_A = \frac{\text{moles A}}{\text{(mole mixture)(sec)}} .$$

Since one is going to consider the liquid phase system, the rate of disappearance of A is given by Equation (20) or by Equation (21).

Chapter III

MATHEMATICAL ANALYSIS OF THE PROCESS

The performance equations of isothermal flow reactors can be derived essentially from a material balance based on any reaction component. For an element of volume (see Figure 11), the material balance can be written as

$$\begin{array}{l}\text{rate of}\\ \text{reactant}\\ \text{flow into}\\ \text{element of}\\ \text{volume}\end{array} = \begin{array}{l}\text{rate of}\\ \text{reactant}\\ \text{flow out}\\ \text{of element}\\ \text{of volume}\end{array} + \begin{array}{l}\text{rate of reactant}\\ \text{loss due to chem-}\\ \text{ical reaction}\\ \text{within the ele-}\\ \text{ment of volume}\end{array} + \begin{array}{l}\text{rate of accu-}\\ \text{mulation of}\\ \text{reactant in}\\ \text{element of}\\ \text{volume}\end{array} \qquad (22)$$

Where the composition within the reactor is uniform (independent of position), the material balance may be made over the whole reactor. Where the composition is not uniform, the balance must be made over a differential element of volume and then integrated subject to appropriate boundary conditions which depend on operating conditions and the geometry of the system.

1. PERFORMANCE OF A STEADY-STATE CONTINUOUS STIRRED TANK REACTOR

Since the composition is uniform throughout a CSTR the material balance may be made considering the reactor as a whole. By selecting reactant A for consideration, Equation (22) becomes, under steady state condition,

Input of A = output of A + dissappearance of A by reaction

or

$$\text{Input of A} - \text{output of A} - \text{dissappearance of A by reaction} = 0 \tag{23}$$

As shown in Figure 12(a) if F is the molal feed rate of a mixture into the reactor, then considering the reactor as a whole, one has

$$\text{Input of A, moles/time} = F(x_{Ao})$$

$$\text{Output of A, moles/time} = F(x_{A_1})$$

$$\begin{array}{l}\text{Dissappearance}\\ \text{of A by reaction,}\\ \text{moles/time}\end{array} = (-r_A)V_1 = \frac{\text{moles A reacting}}{(\text{time})\left(\begin{array}{l}\text{volume of}\\ \text{reacting}\\ \text{fluid}\end{array}\right)}\left(\begin{array}{l}\text{volume of}\\ \text{reactor}\\ \text{occupied by}\\ \text{reacting fluid}\end{array}\right)$$

Substituting these terms in Equation (23), one obtains

$$F(x_{A_0}) - F(x_{A_1}) = (-r_A)V_1$$

which on rearranging becomes

$$(x_{A_0} - x_{A_1}) = (-r_A)\frac{V_1}{F} = (-r_A)\frac{\theta_1}{\rho} \tag{24}$$

where θ_1 = mean holding time of a CSTR = $\frac{V_1}{F}$, sec. (25)

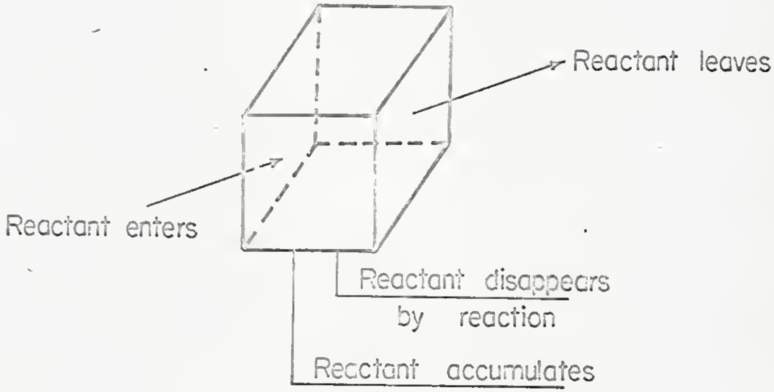
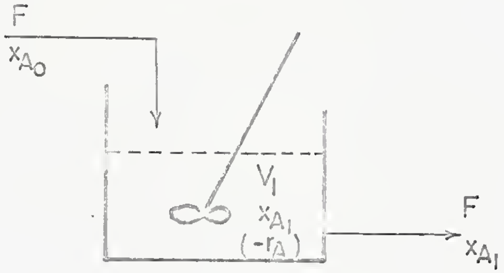
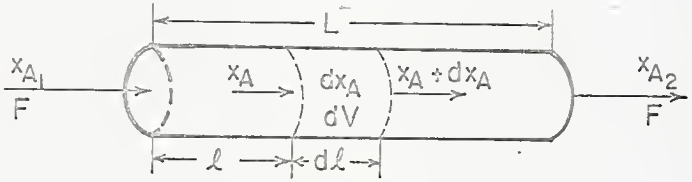


Fig. 11.. The general material balance for a volume dV .



(a). Variables for CSTR



(b). Variables for PFTR

Fig. 12. Variables for CSTR & PFTR.

The rate of disappearance of A is given by Equation (20) and hence Equation (24) becomes

$$x_{A_0} - x_{A_1} = [k_1 \rho x_{A_1} + k_2 \rho^2 x_{A_1} (1-x_{A_1})] \frac{\theta_1}{\rho}$$

Simplification gives the performance equation for a CSTR as

$$x_{A_1} = x_{A_0} - [k_1 x_{A_1} + k_2 \rho x_{A_1} (1-x_{A_1})]\theta_1 \tag{26}$$

2. PERFORMANCE OF A STEADY-STATE PLUG FLOW TUBULAR REACTOR

In a plug flow reactor the composition of the fluid varies with position along a flow path. Consequently, the material balance for a reaction component must be made for a differential element of volume dV. Thus for a component A, one obtains

Input of A = Output of A + Disappearance of A by reaction

Referring to Fig. 12(b), it can be seen that for a volume dV

Input of A, moles/time = $F(x_A)$

Output of A, moles/time = $F(x_A + dx_A)$

where x_A is the fractional conversion of A at inlet of element volume dV, and

Disappearance of A by reaction, moles/time = $(-r_A)dV$.

Substitution of these terms into equation (27) gives

$$Fx_A - F(x_A + dx_A) = (-r_A)dV$$

or

$$-Fdx_A = (-r_A)dV \tag{28}$$

$(-r_A)$ is given by Equation (20) and hence one gets

$$-Fdx_A = [k_1\rho x_A + k_2\rho^2 x_A(1-x_A)]dV$$

where

$$dV = Adl$$

Therefore, the performance equation of the PFTR is

$$dx_A = -(\frac{A\rho}{F})[k_1 x_A + k_2\rho x_A(1-r_A)]dl \tag{29}$$

and

$$x_A = x_{A_1} \quad \text{at} \quad l = 0 \tag{30}$$

3. SUMMARY OF PERFORMANCE EQUATIONS

Following the usual procedure, the equations to be solved on the computer are written for the highest derivative.

For a CSTR

$$x_{A_1} = x_{A_0} - [k_1 x_{A_1} + k_2 \rho x_{A_1} (1-x_{A_1})]\theta_1 \tag{26}$$

For a PFTR

$$\frac{dx_A}{dl} = A - \frac{A\rho}{F} [k_1 x_A + k_2 x_A (1-x_A)] \tag{31}$$

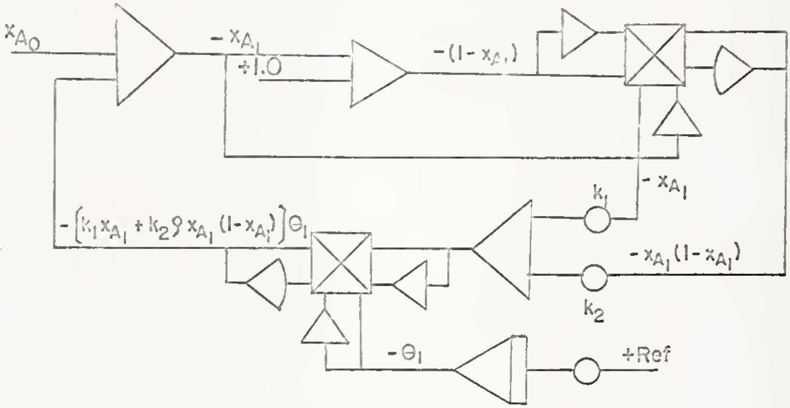
with Initial Condition as $x_A = x_{A_1}$ at $l = 0$, (30)

or

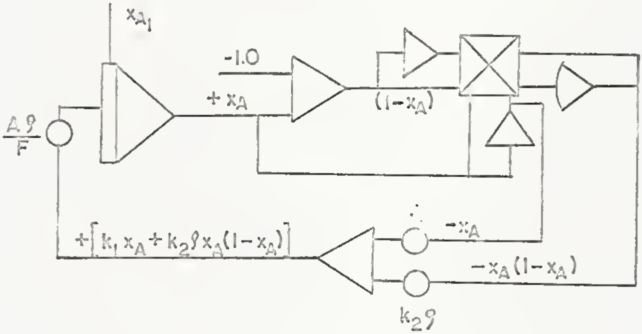
$$\dot{x}_A = \frac{dx_A}{dt} = - \frac{A\rho}{F} [k_1 x_A + k_2 x_A (1-x_A)] \tag{32}$$

with Initial Condition as $x_A = x_{A_1}$ at $t = 0$, (33)

where one unit of reactor length has been changed to one unit of computer time. Unscaled computer diagrams for these two models are shown in Figure 13. In Figure 13(a), one has used an integrator to sweep the θ.



(a). CSTR . $x_{A_1} = x_{A_0} - \left[k_1 x_{A_1} + k_2 \rho x_{A_1}(1-x_{A_1})\right]\Theta_1$



(b). PFTR . $\dot{x}_A \equiv \frac{d x_A}{d l} = \frac{-A\rho}{F}\left[k_1 x_A + k_2 \rho x_A (1-x_A)\right]$

Fig. 13. Unscaled diagrams of CSTR and PFTR.

Chapter IV

SCALING AND STATIC TESTS FOR THE ANALOG COMPUTER

1. MAGNITUDE SCALING

From previous knowledge of this system, the maximum values of some of the variables are predetermined. These maximum values of the variable and typical values of the parameters are given below.*

F = molal feed rate of mixture which remains constant

$$= 5 \frac{\text{moles of mixture}}{\text{sec}}$$

ρ = density of the mixture which also remains constant

$$= 5 \frac{\text{moles of mixture}}{\text{ft}^3}$$

k_1 = reaction rate constant = 10^{-3} sec^{-1}

k_2 = reaction rate constant = $10^{-1} \frac{\text{ft}^3}{\text{moles sec}}$

D = diameter of PFTR = 2.0 ft

x_A = feed mole fraction of A to the CSTR = $1.0 \frac{\text{moles of A}}{\text{moles of mixture}}$

$\theta_{1_{max}}$ = maximum residence time for CSTR = $\frac{V_1}{F}$ = 10 secs.

$x_{A_{max}}$ = maximum mole fraction of A = $1.0 \frac{\text{moles of A}}{\text{moles of mixture}}$

---

*The model is based on a plug flow assumption. Since this solution is not for a particular fluid, this assumption is not important. However, when the model is used for a real system, the Reynolds number of the system must be calculated to check the validity of the model.

$$x_{B\ max} = (1-x_A)_{max} = \text{maximum mole fraction of B}$$

$$= 1.0 \frac{\text{moles of B}}{\text{moles of mixture}}$$

Referring to the summary of equations and the unscaled diagram (Figure 13), the following variables and derivatives will be represented on the computer and will, therefore, require scaling

$$x_{A_0},\ x_{A_1},\ (1-x_{A_1}),\ x_{A_1}\ (1-x_{A_1}),\ [k_1 x_{A_1} + k_2 \rho x_{A_1}\ (1-A_1)], \theta_1,$$

$$[k_1 x_{A_1} + k_2 \rho x_{A_1}\ (1-x_{A_1})]\theta_1,\ \dot{x}_A,\ x_A,\ (1-x_A),\ x_A(1-x_A),$$

$$[k_1 x_A + k_2\ x_A(1-x_A)]$$

The $\dot{x}_A$ is not required explicitly in the results. It can be formed at the input to the integrator and will not, therefore, require scaling as such.

Table I summarizes the magnitude scaling and Table II summarizes the parameter values for the given problem.

2. SCALED EQUATIONS

The scaled equations can now be written by substituting the scaled variables from Table I into the original equations.

For CSTR

$$x_{A_1} = x_{A_0} - \{k_1 x_{A_1} + k_2 \rho x_{A_1}\ (1-x_{A_1})\}\theta_1$$

Table I

Magnitude Scaling for System Variables

Physical Variables	Estimated Maximum Values	Units	Scale Factor $\frac{\text{M.V.}}{\text{E.M.V.}}$	Computer Variables
x_{A_0}	1.0	$\frac{\text{moles A}}{\text{moles mix}}$	1.0	$[x_{A_0}]$
x_{A_1}	1.0	$\frac{\text{moles A}}{\text{moles mix}}$	1.0	$[x_{A_1}]$
$(1-x_{A_1})$	1.0	$\frac{\text{moles A}}{\text{moles mix}}$	1.0	$[1-x_{A_1}]$
$x_{A_1}\ (1-x_{A_1})$	1.0	$\left(\frac{\text{moles A}}{\text{moles mix}}\right)^2$	1.0	$[x_{A_1}\ (1-x_{A_1})]$
$k_1x_{A_1} +$ $k_2\rho x_{A_1}\ (1-x_{A_1})$	0.2	$\frac{\text{moles A}}{\text{(moles mix)sec}}$	5.0	$[5k_1x_{A_1} +$ $5k_2\rho x_{A_1}\ (1-x_{A_1})]$
θ_1	10	sec	0.1	$[.1\theta_1]$
$\{k_1x_{A_1} +$ $k_2\rho x_{A_1}\ (1-x_{A_1})\}\theta_1$	2.0	$\frac{\text{moles A}}{\text{moles mix}}$	0.5	$[[5k_1x_{A_1} +$ $5k_2\rho x_{A_1}(1-x_{A_1})][0.1\theta_1]]$
$\dot{x}_A$	1.0	$\frac{\text{moles A}}{\text{moles mix,sec}}$	1.0	$[\dot{x}_A]$
x_A	1.0	$\frac{\text{moles A}}{\text{moles mix}}$	1.0	$[x_A]$
$(1-x_A)$	1.0	$\frac{\text{moles A}}{\text{moles mix}}$	1.0	$[1-x_A]$
$X_A(1-x_A)$	1.0	$\left(\frac{\text{moles A}}{\text{moles mix}}\right)^2$	1.0	$[x_A(1-x_A)]$
$k_1x_A +$ $k_2\rho x_A(1-x_A)$	0.2	$\frac{\text{moles A}}{\text{(moles mix)sec}}$	5.0	$[5k_1\ x_A +$ $5k_2\ \rho x_A(1-x_A)]$

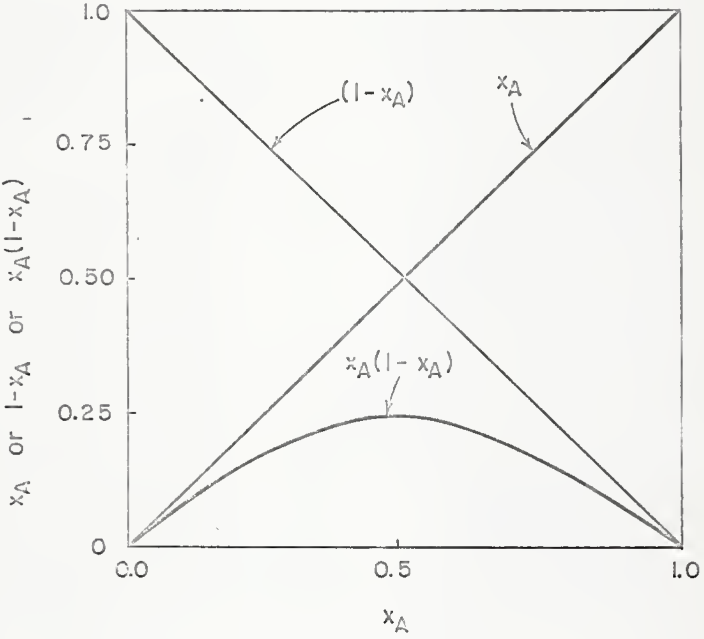


Fig. 14. Expected maximum values of $x_A(1-x_A)$.

Table II

Parameter Summary

$F = 5 \ \frac{\text{moles of mixture}}{\text{sec}}$

$\rho = 5 \ \frac{\text{moles mixture}}{\text{ft}^3}$

$k_1 = 10^{-3} \ \text{sec}^{-1}$

$k_2 = 10^{-1} \ \frac{\text{ft}^3}{\text{moles sec}}$

$D = 2.0$ ft

$x_{A_0} = 1.0 \ \frac{\text{moles of A}}{\text{moles of mixture}}$

$$\therefore\ [x_{A_1}] = [x_{A_0}] - \frac{1}{0.5}\{[5k_1 x_{A_1} + 5k_2\ x_{A_1}\ (1-x_{A_1})][0.1\theta_1]\}$$

or

$$[x_{A_1}] = [x_{A_0}] - 2.0\ \{[\frac{1}{10}\ (50k_1)x_{A_1} + 10(\frac{5k_2\rho}{10})x_{A_1}\ (1-x_{A_1})][.1\theta_1]\} \tag{34}$$

<u>For PFTR</u>

$$\frac{dx_A}{dt} = \dot{x}_A = -\frac{A\rho}{F}\{k_1 x_A + k_2 \rho x_A (1-x_A)\}$$

$$\therefore\ [\dot{x}_A] = -\frac{A\rho}{5F}\ [5k_1 x_A + 5k_2 \rho x_A (1-x_A)]$$

$$\therefore\ [\dot{x}_A] = -\ (\frac{A\rho}{5F})\ [\frac{1}{10}\ (50k_1)x_A + 10(\frac{5k_2\rho}{10})x_A(1-x_A)] \tag{35}$$

and I. C. is $[x_A] = [x_{A_1}]$ at $t = 0$. (36)

3. TIME SCALING

Equation (35) can be written as

$$[\dot{x}_A] = -\ (\frac{A\rho}{5F\beta})\ [\frac{1}{10}\ (50k_1)x_A + 10\ (\frac{5k_2\rho}{10})\ x_A(1-x_A)] \tag{37}$$

where $\beta = 1.0$, i.e., 1 unit time of computer = 1 unit length of PFTR.

The scaled diagram is drawn as in Figure 15 using Equations (34), (36), and (37).

4. STATIC TEST

The introduction of initial condition voltages (IC-voltages) into the circuit permits the calculation of output and checkpoint voltages to be expected on the amplifiers and integrators. The IC-voltages, which will be chosen for convenience for static test, need not have any physical significance. The outputs and checkpoints will be calculated from the original equations, to insure that errors have not been made either in the scaled equations or in the mechanization.

Check Calculations:

1. Since the performance equation of the CSTR is the algebraic equation, one can calculate x_{A_1} as follows.

$$x_{A_1} = x_{A_0} - [k_1 x_{A_1} + k_2 \rho x_{A_1} (1 - x_{A_1})]\theta_1$$

where

$x_{A_0} = 1.0$, moles A/moles of mixture

$\rho = 5.0$, moles mixture/ft^3

$k_1 = 10^{-3}$, sec^{-1}

$k_2 = 10^{-1}$, ft^3/moles (sec)

$\theta_1 = 100$, secs.

Hence substitution of these terms into the above expression gives

$$50x_{A_1}^2 - 51.1x_{A_1} + 1 = 0$$

$$\therefore x_{A_1} = 0.511 \pm 0.491$$

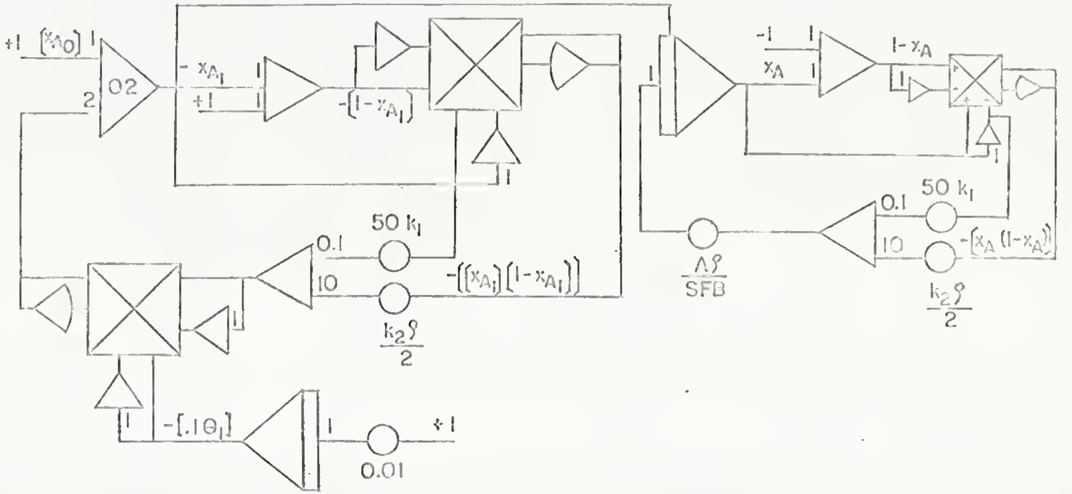


Fig. 15. Scaled diagram for CSTR and PFTR.

$$x_{A_1} = [x_{A_0}] - 2\left\{\left[\frac{1}{10}(50k_1)x_{A_1} + 10\left(\frac{k_2 \rho}{2}\right)x_{A_1}(1-x_{A_1})\right][0.1\theta_1]\right\}$$

$$\frac{d[x_A]}{d\ell} = -\left(\frac{A\rho}{SF\beta}\right)\left[\frac{1}{10}(50k_1)x_A + 10\left(\frac{k_2 \rho}{2}\right)x_A(1-x_A)\right]$$

$$x_A = x_{A_1} \quad \text{at} \quad \ell = 0$$

Since A is consumed in the CSTR, x_{A_1} must be less than one and hence, one obtains

$$x_{A_1} = 0.02.$$

2. $\dot{x}_A = - \frac{A\rho}{F} \{k_1 x_A + k_2 \rho x_A \ (1-x_A)\}$

$D = 2.0$, ft

$F = 5.0$, moles mixture/sec

Hence,

$$\dot{x}_A = - \frac{(\pi)(4)(5)}{(4)(5)} 10^{-3} \ (0.02) + 10^{-1} \ (5)(.02)(.98)$$

or

$$\dot{x}_A = - 0.03$$

3. The output voltages of individual amplifiers and pots are shown in Tables III and IV.

Table III

TR-48 Potentiometer Assignment Summary for Figure 14

Parameter Description	Setting Static Check Voltage	Static Check Output Voltage	Setting Run Number 1	Notes
I.C. on θ_1	1.0	1.0	0.0	Disconnect
Constant	0.01	0.01	0.01	
$50k_1$	0.05	-0.001	0.05	
$k_2\rho/2$	0.25	-0.0049	0.25	
$A\rho/5F$	0.628	0.0309	0.628	
$50k_1$	0.05	-0.001	0.05	
$k_2\rho/2$	0.25	-0.0049	0.25	

Table IV

TR-48 Amplifier Assignment Summary for Figure 14

FB	OUTPUT VARIABLE	STATIC CHECK			
		CALCULATED		MEASURED	
		Deriv.	Output	Deriv.	Output
ε	$-[x_{A_1}]$	--	-0.02	--	-0.019
ε	$-[1-x_{A_1}]$	--	-0.98	--	-0.98
ε	$[5k_1x_{A_1} + 5k_2\rho x_{A_1}(1-x_{A_1})]$	--	0.049	--	0.049
∫	$-[0.1\theta_1]$	0.01	-1.0	-0.01	-1.0
I	$[1-x_{A_1}]$	--	+0.98	--	0.98
I	$[x_{A_1}]$	--	0.02	--	0.02
I	$-[5k_1x_{A_1} + 5k_2\rho x_{A_1}(1-x_{A_1})]$	--	-0.049	--	-0.05
I	$[0.1\theta_1]$	--	+1.0	--	1.0
H	$-[5k_1x_{A_1} + 5k_2\rho x_{A_1}(1-x_{A_1})][.1\theta_1]$	--	-0.049	--	-0.05
H	$-[x_{A_1}(1-x_{A_1})]$	--	-0.0196	--	-0.019
∫	x_A	-0.0309	0.02	0.03	0.02
ε	$1-x_A$	--	0.98	--	0.98
ε	$[5k_1x_A + 5k_2\rho x_A(1-x_A)$	--	0.049	--	0.05
I	$-[1-x_A]$	--	-0.98	--	-0.98
I	$-[x_A]$	--	-0.02	--	-0.02
H	$[x_A(1-x_A)]$	--	-0.0196	--	-0.0196

Chapter 5

RESULTS AND CONCLUSIONS

The output concentration of A, x_{A_1}, from the CSTR is plotted against the mean holding time, θ_1, of the CSTR in Figure 15. It is useful because for a given mean holding time θ_1 the corresponding x_{A_1} can be read from it, or vice versa. Also, it has been observed that the algebraic circuit of the CSTR on the analog computer becomes unstable as soon as θ_1 reaches approximately 5.5 secs. Since it has been anticipated that the maximum θ_1 would be in the range of 10 seconds, a more stable algebraic circuit is needed on the analog computer. To eliminate the instability of the algebraic part of the circuit as θ_1 goes beyond 5.5 seconds, the amplifier 02 in the Figure 14 is replaced by an integrater. This then represents an unsteady state performance equation circuit for the CSTR, but if the rate of integration is fast compared to the rate of change of mean holding time, θ_1, then the circuit will approximately be at steady state at all times. This integrator 02 should be patched in such a manner that when the computer is in the rep-op (repetitive operation) mode then it will be in the operate mode and also the β plug should be removed for faster integration.

The unsteady-state material balance on A around the CSTR gives the following scaled and unscaled performance equations.

Accumulation of A = Input of A - Output of A - Conversion of A

$$\frac{dx_1}{dt} = Fx_{A_0} - Fx_{A_1} - F[k_1 x_{A_1} + k_2 \rho x_{A_1} (1-x_{A_1})]\theta_1 \qquad (21)$$

and

$$\frac{d[x_1]}{dt} = 10\left(\frac{F}{10}\right)[x_{A_1}] - 10\left(\frac{F}{10}\right)[x_{A_1}] - 10\left(\frac{F}{5}\right)\left[\left[\frac{1}{10}(50k_1)x_{A_1} + 10\left(\frac{k_2\rho}{2}\right) x_{A_1}(1-x_{A_1})\right][.1\theta_1]\right] \qquad (22)$$

Using the integrator 02 instead of amplifier 02 in the Figure 14, x_{A_1} is plotted against θ_1 as shown in Figure 16 as before. It can be seen from Figure 16a that the circuit is stable for beyond 10 seconds to approximately 12 seconds. The accuracy of this unsteady state approximation can be estimated by superimposing Figure 16 on 16a. This shows that the approximation by unsteady state performance equation for the steady state CSTR is quite reliable except for very rapid changes in x_{A_1}.

Next the conversion of A in the PFTR at any distance from the entrance or at any time from the entrance is plotted in Figure 17. This is repeated for different initial feed compositions of A, i.e., for different values of x_{A_1}. The required length of the PFTR, L, and mean holding time of the PFTR, θ_2, for a desired conversion and for a given initial feed composition can now be found.

Table 5 is prepared from Figures 16 and 17. Using Table 5, the total mean holding time of the system can be plotted against the mean holding time of the CSTR as shown in Figure 18. It can be noted from Figure 18 that for a desired 80% conversion of A, there is a minimum total mean holding time of the system and a particular corresponding mean holding time of the CSTR. One can repeat the same procedure for

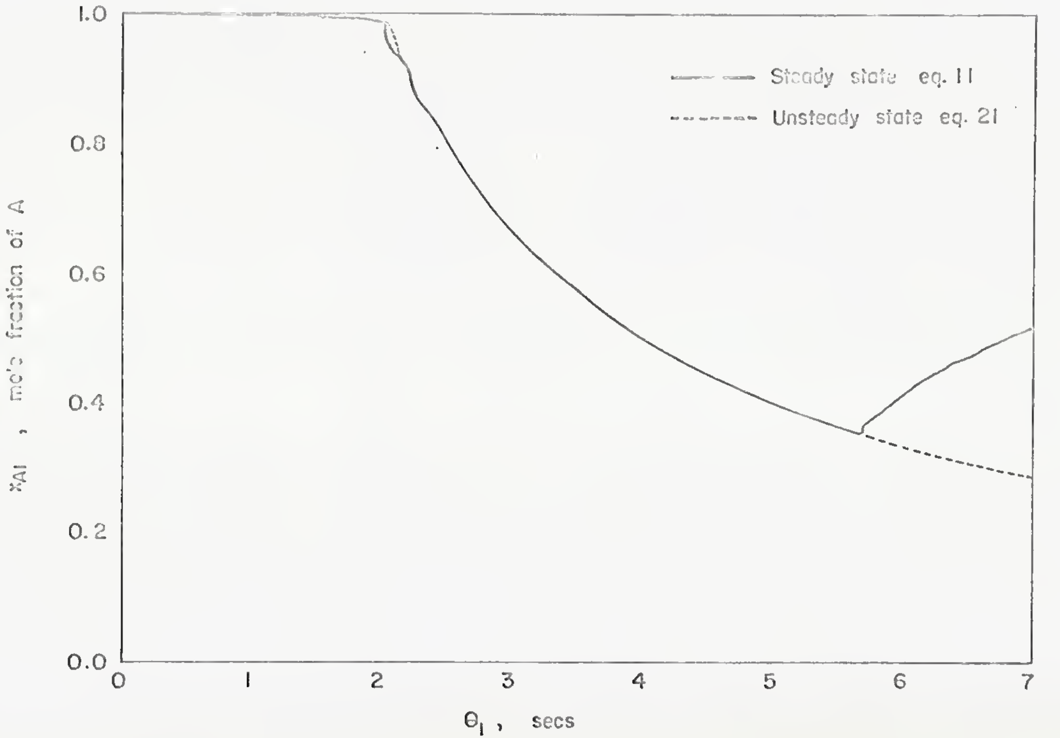


Fig. 16. Output concentration of A from CSTR vs. mean holding time of CSTR.

different conversions and get the corresponding minimum total mean holding time ($\theta_1 + \theta_2$) and also the corresponding θ_1. This requires considerable amount of calculation and effort; therefore, it has been decided to use the same procedure on the analog computer.

To accomplish this the comparator and track/store units of the computer are utilized. The final analog computer diagram is shown in Figure 19. The comparator, in Figure 19 compares the desired conversion with the conversion in the PFTR at any instant and sends binary signals to track and store units, respectively. When the conversion in the PFTR has reached the desired conversion then the signals are reversed interchanging track and store units.

Integrator 21 generates the time on the computer which is directly proportional to the length of the PFTR. If one denotes the time generated by integrator 21 as t_2, then t_2 is proportional to the length ℓ of the PFTR. Now, if τ is the time from entrance of the PFTR to any point in the PFTR of the material, then

$$\tau = \frac{\ell}{v}$$

where v is the velocity of the material in the PFTR and hence

$$v = \frac{F}{A\rho} = \frac{5}{\frac{\pi 4}{4}\,5} = \frac{1}{\pi}\ ,\ \text{ft/sec}$$

Substituting this value of velocity in the above expression gives

$$\tau = \pi\ell,\ \text{secs} \qquad (23)$$

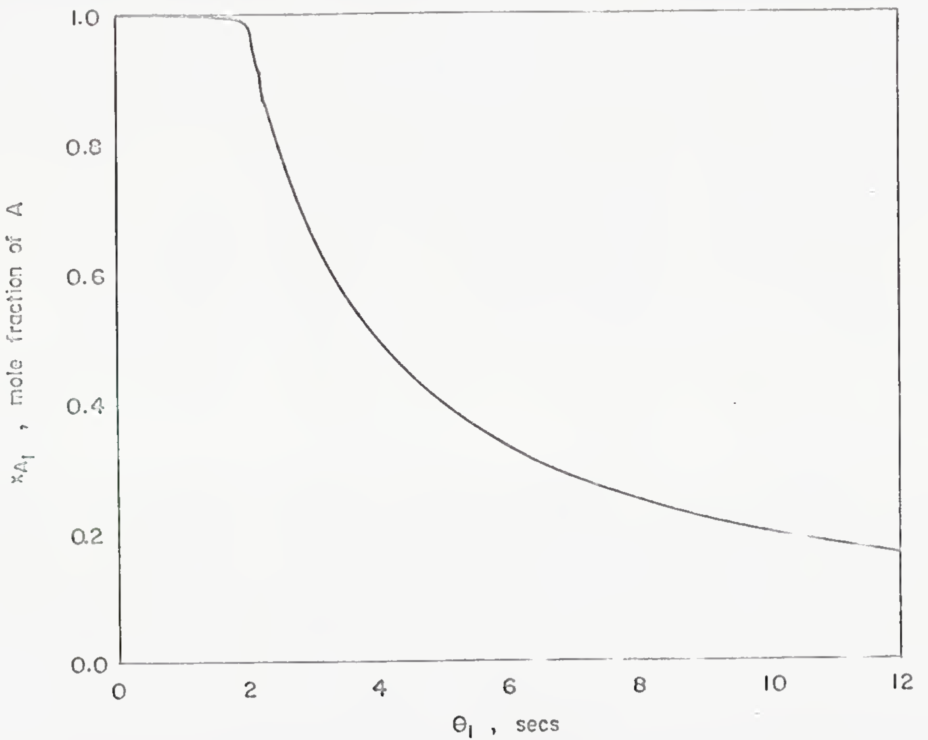


Fig. 16a. Output concentration of A from CSTR vs mean holding time of CSTR using unsteady state eqn. 21 .

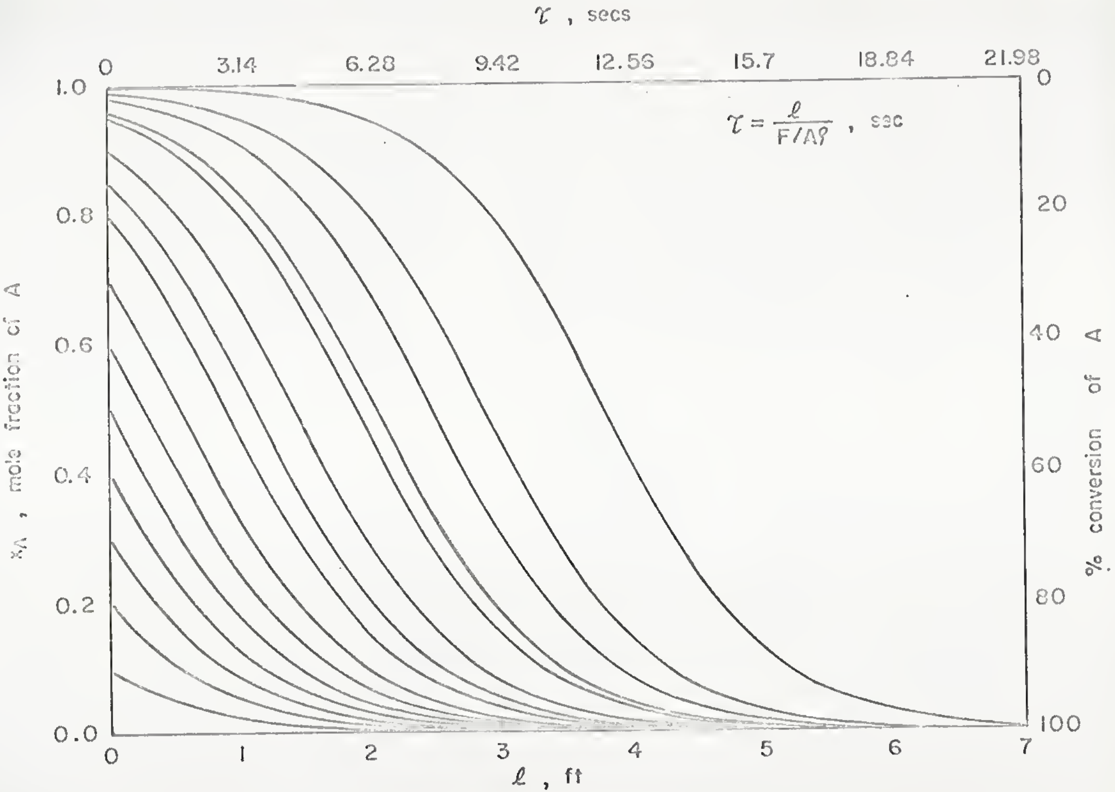


Fig. 17. Conversion of A in PFTR vs length from entrance and time from entrance of PFTR.

Table V

Total Mean Holding Time of the System for a Given Conversion of 80%

Feed Composition of A for PFTR x_{A_1}	Length of PFTR for 80% conversion of A L, ft	Mean holding time of PFTR for 80% conversion θ_2, secs.	Mean holding time of CSTR for 80% conversion θ_1, secs.	Total mean holding time $(\theta_1+\theta_2)$ secs.
1.00	4.65	14.6	0.00	14.60
0.99	3.74	11.7	2.00	13.70
0.98	3.35	10.5	2.05	12.55
0.96	2.90	9.10	2.10	11.20
0.95	2.76	8.66	2.11	10.77
0.90	2.30	7.00	2.25	9.25
0.85	2.00	6.28	2.35	8.63
0.80	1.80	5.65	2.50	8.15
0.70	1.45	4.55	2.85	7.40
0.60	1.15	3.61	3.35	6.96
0.50	0.9	2.82	4.00	6.82
0.40	0.65	2.04	5.00	7.04
0.30	0.35	1.10	6.65	7.75
0.20	0.0	0.0	10.00	10.00

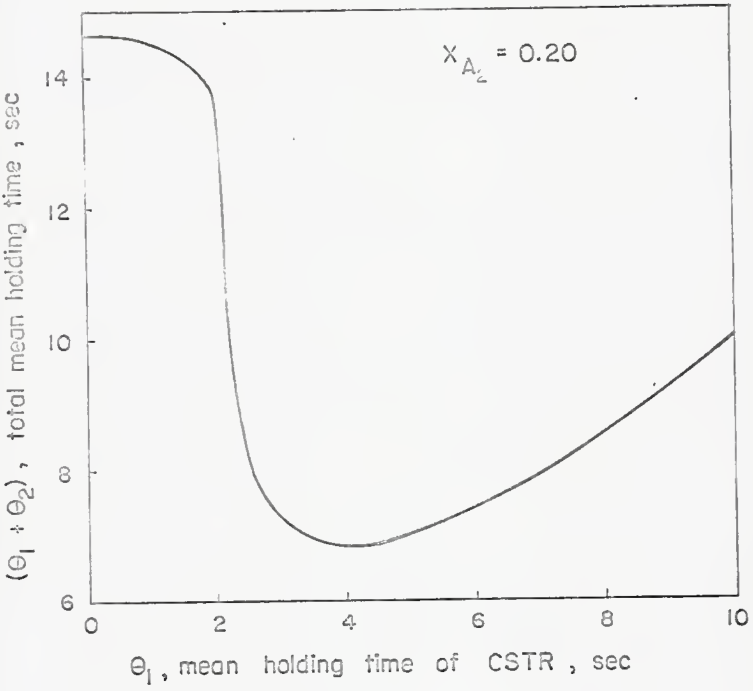


Fig. 18. Total mean holding time of the system $(\Theta_1 + \Theta_2)$ vs the mean holding time of CSTR.

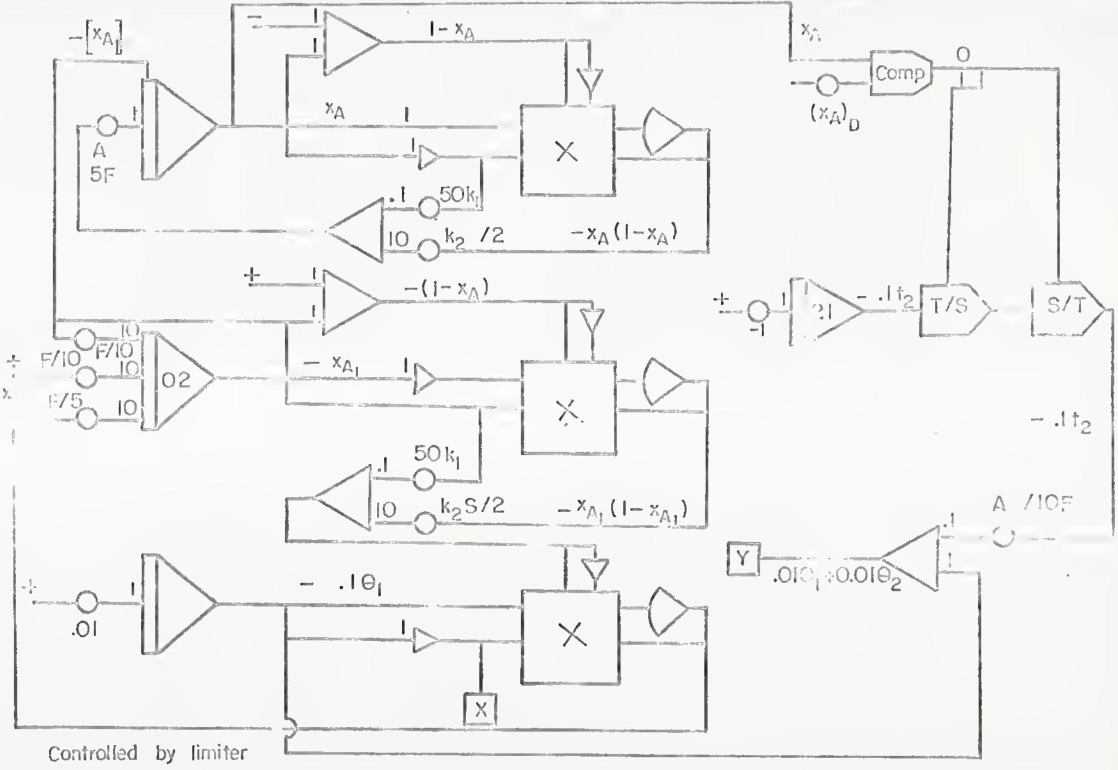


Fig. 19. Complete scaled diagram of CSTR and PFTR.

and when

$$\ell = L$$

then one has $\tau = \theta_2$, and this is equal to t_2, the time generated by integrator 21.

A typical set of computer results are presented in Figures 20 and 21. In Figure 20, the total mean holding time of the system is plotted against the mean holding time of the CSTR for different conversions. It can be seen that a set of curves similar to the curve resulting from hand calculation in Figure 18 has been obtained. It is noted from Figure 18 that for an 80% conversion of A the minimum mean holding time is approximately 6.8 seconds, while it is noted in Figure 20 that for the same conversion the minimum mean holding time is approximately 6.6 seconds. Hence the analog computer technique is a good approximation to the accurate hand or digital calculation technique. The locus of the minimum mean holding times for different conversions is also drawn in Figure 20. Since the curves are very flat, it is hard to determine the accurate minimums in the diagram. It is also seen from Figure 20 that none of the curves cut the line where θ_2 is equal to zero (that is, all conversion in the tank), which is physically realistic since negative θ_2 is not possible.

In Figure 21, the total mean holding time of the system for an 80% conversion of A is plotted against the mean holding time of the CSTR with β (the ratio of the two rate constants, that is, $\beta = \frac{k_2}{k_1}$) as

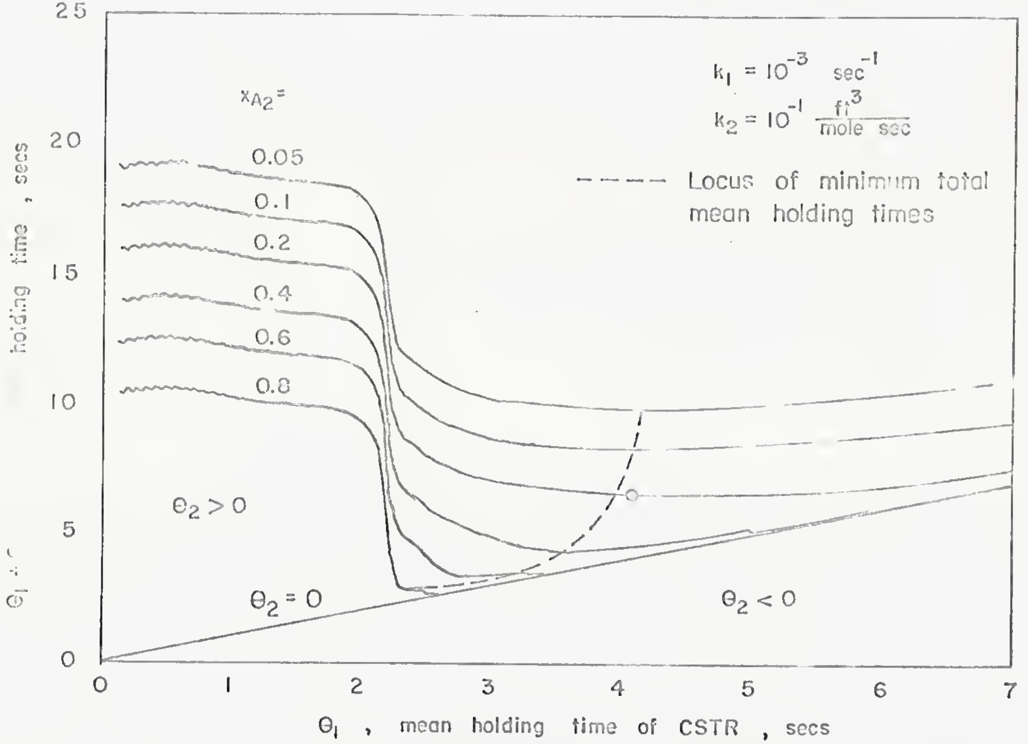


Fig. 20. Total mean holding time vs. mean holding time of CSTR for a given rate constants and x_{A_2} as parameters.

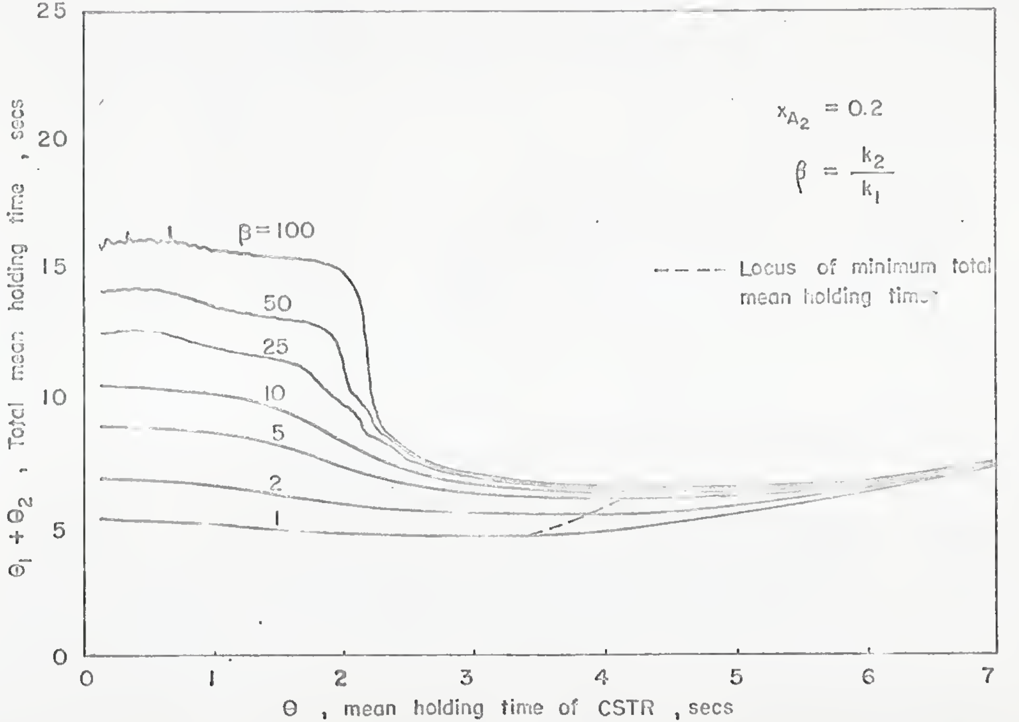


Fig. 21. Total mean holding time vs. mean holding time of CSTR for a given conversion and β as parameter.

a parameter. It is observed from Figure 21 that for β between 25 and 100 the minimum mean holding time of the system and the corresponding mean holding time of the CSTR are affected very little by β. In general, however, the minimum total mean holding time of the system decreases with decreasing β. As β becomes smaller and smaller, the reactions become less and less autocatalytic. When $\beta=1$, this is the case where the rates of initiating reaction and autocatalytic reaction are equal and B is used up as soon as it forms. Hence, the two reactions (Equations (15) and (16)) can appear as one reaction

$$A \rightarrow 2B,$$

which is very similar to the non-catalytic reaction. Also note that the minimum becomes much less pronounced as β approaches one.

In conclusion it can be said that for a desired conversion there is a minimum total mean holding time (or a minimum total volume) of the system and also there is a corresponding mean holding time of the CSTR. One should bear in mind that these results are true if and only if the assumption of plug flow is closely realized in the tubular reactor.

NOMENCLATURE

SYMBOLS

F	Inlet molal feed rate, $\frac{\text{moles}}{\text{sec}}$
x_{A_o}	Feed mole fraction of component A to the CSTR $\frac{\text{moles of A}}{\text{moles of mixture}}$
x_{B_o}	Feed mole fraction of component B to the CSTR $x_{B_o} = 1 - x_{A_o}$
x_{A_1}	Outlet mole fraction for CSTR of component A Inlet mole fraction for PFTR of component A
x_{B_1}	Outlet mole fraction for CSTR of component B $x_{B_1} = (1 - x_{A_1})$ Inlet mole fraction for PFTR of component B
x_{A_2}	Outlet mole fraction for PFTR of component A
x_{B_2}	Outlet mole fraction for PFTR of component B, $x_{B_2} = 1 - x_{A_2}$
x_A	Fractional mole conversion of A at any time
k_1	Reaction rate constant, 1/sec
k_2	Reaction rate constant, $\frac{(\text{ft})^3}{\text{moles, sec}}$
r	Reaction rate, $\frac{\text{moles}}{\text{ft}^3\ \text{sec}}$
C_A	Concentration of component A, moles/ft^3
C_B	Concentration of component B, moles/ft^3
V_1	Volume of CSTR, ft^3
V_2	Volume of PFTR, ft^3

A	Cross-sectional area of PFTR, ft^2
D	Diameter of PFTR, ft
L	Length of PFTR, ft
l	Length from the entrance of PFTR, ft
θ_1	Mean holding time for CSTR, sec
θ_2	Mean holding time for PFTR, sec
τ	Time from the entrance of PFTR, sec
t_2	Computer time which is proportional to length of PFTR, sec
ρ	Density of mixture, $\frac{\text{moles mixture}}{ft^3}$

PART II

DYNAMIC STUDY OF WASTE WATER TREATMENT AND ITS PROCESSES

Chapter I

INTRODUCTION

1. BIOCHEMICAL ENGINEERING AND CHEMICAL ENGINEERING

Various definitions of biochemical engineering have been given. H. Hartley (11) has stated "Biochemical engineering is the practical application of our knowledge of microorganisms. The industrial application of a biochemical process is a combined operation in which the biochemist, the microbiologist, the geneticist, and the chemical engineer are all intimately concerned." In lectures on biochemical engineering at the University of Tokyo in 1963, the following definition was offered: "Biochemical engineering is that activity concerned with economic processing of materials of biological character or origin to serve useful purposes. The function of the biochemical engineer is that of translating the knowledge of the microbiologist and the biochemist into a practical operation."

From the foregoing definitions, it is obvious that biochemical engineering is intimately related to chemical engineering. A biochemical engineer must not only have an appreciation of the biological science, but he also must be well grounded in chemical engineering principles.

2. OBJECTIVES IN WASTE WATER TREATMENT AND ITS PROCESSES (30)

Municipal and industrial wastes are treated to protect public health, to avoid nuisance, to prevent the polluting of natural water and of industrial water, and to avoid damage suits. The pollutional characteristics of waste waters may be classified according to their state (suspended, collidal, and dissolved) and their nature (inorganic, organic, gases, and living organisms). However, the major components of organic wastes are usually the suspended solids and the organic content. The treatment of the waste is usually carried out in four steps, viz. pretreatment, biological oxidation, sludge treatment, and disposal.

Pretreatment includes screening, grit removal, and sedimentation or flotation. Biological oxidation is usually accomplished in either fixed-bed units (trickling filters) or in fluid-bed systems (activated sludge or an aerated lagoon). It is employed in removing the colloidal and dissolved organic matter and it also plays the most important role in waste treatment. Sludge from the foregoing units requires further treatment, digestion and dewatering before disposal. Let us consider a complete treatment plant as shown in Figure 1. Generally, the activated sludge process or aerated lagoon process (activated sludge process without a recycle) is a part of such a plant. The primary settling tank removes settleable solids from the raw waste-stream. The settled solids are diverted for stabilization, often by anaerobic digestion. The waste stream from primary settling enters the aeration phase where the organic matter becomes the food source for aerobic microorganisms. The organisms convert a part of the total food energy to biological cell mass (this is the synthesis step) which remains in the liquid stream leaving the aeration tank. The remaining fraction

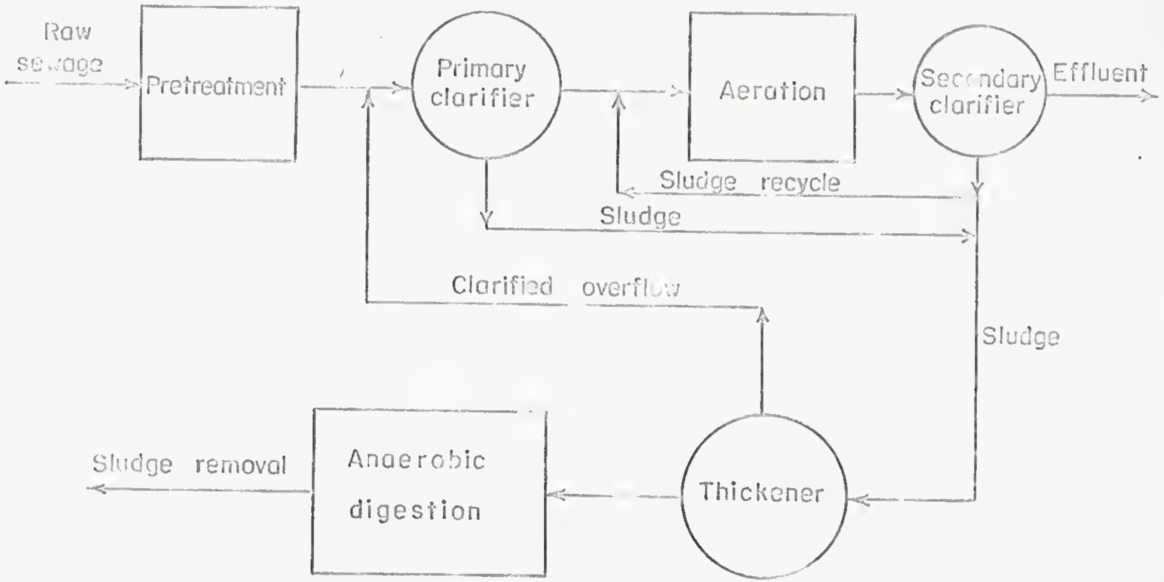


Fig. 1. Waste disposal system by anaerobic digestion.

of the total food is utilized by the organisms as a source of energy for cell synthesis and maintenance. The latter fraction of the food is converted to carbon dioxide and water. The settleable biological solids and inerts are removed from the waste stream in the final settling tank. In the case of the activated sludge process a part of the activated sludge is returned to the aeration tank to maintain a favorable biological solids concentration there while in the case of the aerated lagoon process there is no recycle of activated sludge. The excess solids must be stabilized further, often by anaerobic digestion.

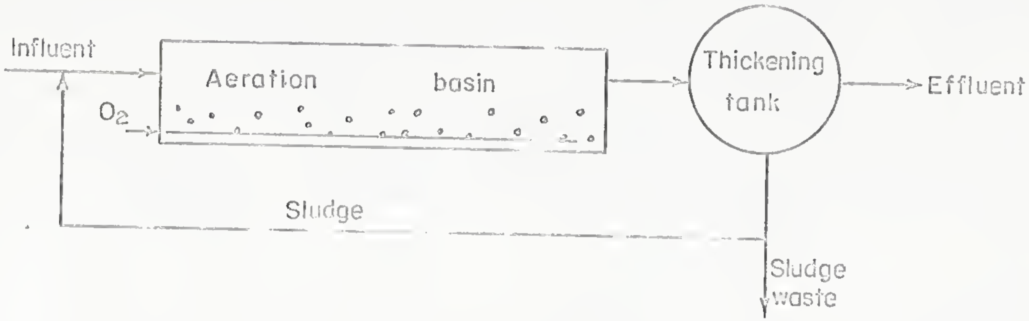
3. WASTE WATER TREATMENT PROCESSES

a. Activated Sludge Process

The activated sludge process may be defined as a system in which flocculated biological growths are continuously circulated and contacted with organic waste in the presence of oxygen. The oxygen is usually supplied from air bubbles injected into the sludge-liquid mass. The process involves an aeration step followed by a solid-liquid separation step from which the separated sludge is recycled back and mixed with the incoming waste. A portion of this sludge is removed for further treatment and disposal. The aeration step may be considered in three functional phases as follows (12):

(1) A rapid adsorption of waste substrate by the activated sludge.

(2) Progressive oxidation and synthesis of the absorbed organics.



g. 2 . Flow diagram of conventional activated sludge process.

(3) Further aeration resulting in oxidation and dispersion of the sludge particles.

Various modifications of the activated sludge process have been developed to achieve economic advantage in construction and operation (13). The conventional activated sludge process as shown in Figure 2 is one of the basic activated sludge processes. The present knowledge concerning the treatment has been summarized very effectively by Haseltine (14).

b. The Aerated Lagoon Process

In the activated sludge process if the separated sludge is not recycled to mix with the incoming waste, then it is known as an aerated lagoon process. This process is mainly used for treatment of feedlot wastes and wastes from refineries. The purpose of lagoons is the destruction and stabilization of organic matter rather than water purification.

4. PROCESS DYNAMICS AND SIMULATION (31)

Microbial systems are inherently dynamic. When the population of organisms changes in a simple shake flask culture, changes are induced in nutrients, viscosity, dissolved oxygen and carbon dioxide, waste products, pH, cell morphology, and just about every other factor. Similarly the complex mixed culture processes for biological treatment of domestic or industrial wastes commonly undergo changes and these can be extreme when shock loads are applied.

Bioengineering must appreciate the dynamic aspects of waste water treatment processes so that design, control, and operation can be optimized. Some of these dynamic aspects are: how the systems fluctuate, how upsets and responses are related, how an organism responds to its environment. In other words, it is important to work out magnitude and time relationships between the factors sensed by microorganisms and the responses to these factors.

Powerful mathematical approaches have been developed for system analysis (32). Mathematical models which can be simulated on computers enable us to evaluate systems characteristics more rapidly than laboratory experiments with living cultures. Constructing the models forces the investigator to develop and understand his systems well. In this work, a mathematical model for the continuously operated bioreactor system has been developed. The transient behavior of this model system under various operating conditions has been simulated on a EAI TR-48 analog computer.

Chapter II

MATHEMATICAL ANALYSIS OF THE SYSTEM

1. THE PRINCIPAL OF AERATION AND A KINETIC MODEL

a. Principle of Biological Oxidation (15)

Biological oxidation is simply a conversion process wherein dissolved organic compounds are converted into bacterial cells, which can then be removed from the waste water. The generalized reaction for the removal of soluble organics may be considered as follows:

$$\text{Organics} + O_2 + \text{Nutrients} \longrightarrow CO_2 + H_2O + \text{Organisms.}$$

In addition to this, some of the organisms die and become inert material in the system, that is,

$$\text{Organisms} + O_2 \longrightarrow CO_2 + H_2O + \text{Inert.}$$

This is referred to as an endogeneous respiration.

b. The Growth of Bacteria (16)

Although growth is usually defined simply as the addition of new substance to individual cells or organisms, the growth of bacteria is actually a complex phenomenon representing the sums of the processes of metabolism.

The term growth is properly applied only to an individual organism. Among bacteria, growth occurs by a certain sequence of events. The individual cell increases in size for a period and then divides into two individuals, each of which can repeat the same process of size increase and binary division. Some hereditary or internal mechanism which is not as yet well understood apparently limits the size of the individual cell.

c. The Growth Pattern (12, 16)

In studying the development of batch bacterial cultures, the classical approach has been to divide the batch growth curve into a series of phases on the basis of changes in the growth rate as shown in Figure 3. Although the boundaries between the phases are usually located at definite points of inflection in the time-growth curves, the phases chosen and described by different workers have not always been the same. For this discussion one will use the phases as described by Monod (17). In Figure 3, these are:

(1) Lag Phase (initial stationary phase),
(2) Acceleration Phase (phase of positive growth acceleration),
(3) Logarithmic growth phase (exponential phase),
(4) Retardation phase (phase of negative growth acceleration),
(5) Stationary phase (maximum stationary phase),
(6) Logarithmic death phase or Endogeneous phase.

From these phases a rather generalized picture of the bacterial growth cycle is drawn. In individual cases any one, or even several of these phases may be absent, and occasionally a more complex pattern of growth is observed.

Each of these phases will now be considered briefly. More thorough discussions of the growth phases may be found in books by Porter (18), Clifton (19) and in the review by Monod (17).

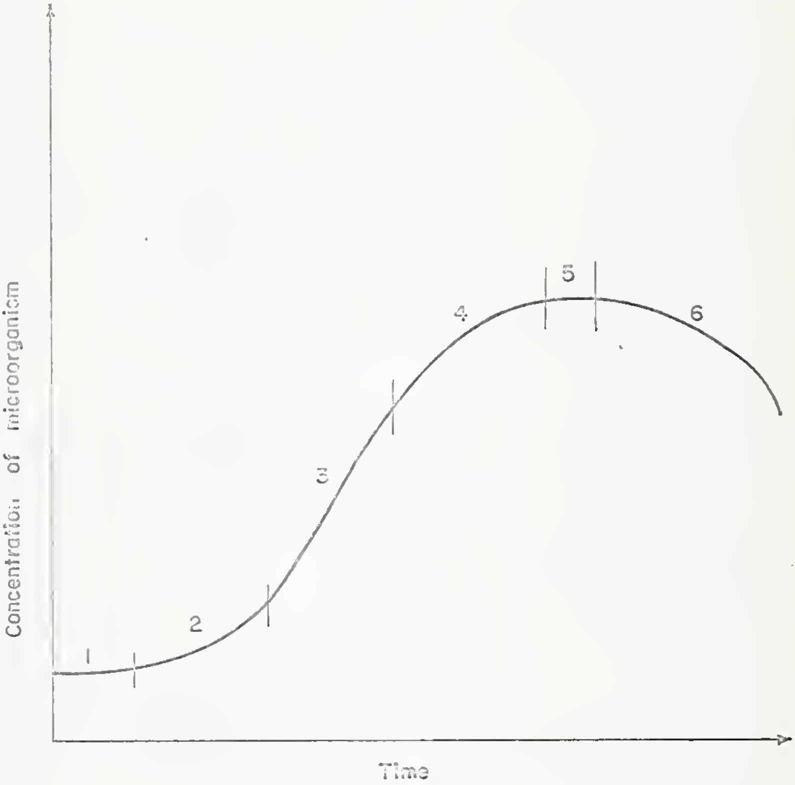


Fig. 3. A typical batch growth curve.

1. The Lag Phase

When transferred into a new medium, the bacterial population often remains constant for a period of time which may be extremely short or may last for hours before an increase can be detected. Occasionally, a temporary decrease in population occurs.

2. The Acceleration Phase

After the initial stationary phase the culture begins to develop; several generations, however, are required before the organisms have completely adjusted themselves for growth and multiplication at a maximal rate in the particular new environment.

3. Logarithmic Phase

The growth is unrestricted since all nutrients are present in excess of the requirements of the microorganism. During this period the growth is constant and the concentration of microorganisms increases at an exponential rate.

4. Retardation Phase

At some concentration, one of the nutrients becomes growth limiting and the culture proceeds into the declining growth phase. In response to the increasing competition of the microorganisms for the remaining limiting nutrient, the rate of growth decreases until growth finally halts.

5. The Stationary Phase

The stationary phase comprises the period during which the bacterial population appears to remain constant at a maximum level.

6. The Death Phase

The remaining position of the curve represents the decrease of the microorganism resulting from autooxidation which occurs after the depletion of the available organics. This is often called the endogeneous respiration phase of waste water treatment processes.

d. Kinetic Model (30, 33)

In an aerobic environment not limited by mixing or nutrients, the specific growth rate is proportional to the concentration of organisms. The mathematical model, therefore, can be represented by

$$r = \frac{dx_2}{dt} = \mu x_2 \qquad (1)$$

where

r = growth rate, mg/liter, hr.,

x_2 = concentration of organisms, mg/liter,

μ = growth rate constant, hr^{-1}.

Monod (17), in his study of bacterial growth in a chemostat (continuous culture), found that his data behaved in a manner typified by Michaelis-Menten equation which is one of the most widely accepted models of enzyme kinetics (33). He therefore suggested the following form for the growth rate constant.

$$\mu = k \left\{\frac{x_1}{K + x_1}\right\} \qquad (2)$$

where

k = specific reaction rate constant which is equivalent to the maximum growth rate when the organic concentration is not limiting the rate of growth, hr^{-1},

K = parameter (a constant) in a kinetic model which is equivalent to the concentration of organics at which the specific growth rate observed is one half the maximum value; saturation constant, mg/liter,

x_1 = concentration of organics, mg/liter.

It is worth noting that when x_1 approaches infinity, that is, when the organic concentration is not limiting, one gets from Equation (2)

$$\mu_{max} = k$$

This expression is precisely the same as the definition of k given above. It is also noted that when K is equal to organic concentration, x_1, in Equation (2), one has

$$\mu = k \left\{\frac{x_1}{x_1 + x_1}\right\}$$

or

$$\mu = \frac{1}{2} k$$

Since

$$\mu_{max} = k$$

one has

$$\mu = \frac{1}{2} k = \frac{1}{2} \mu_{max}$$

Hence, whenever K is equal to organic concentration, x_1, one will always have $\mu = \frac{1}{2} k$ and this is precisely the same definition of K as given above. Then, if one milligram of organics produces Y milligrams of organisms, the rate of consumption of organics will be

$$r_s = -\frac{r}{Y} \tag{3}$$

From an engineering viewpoint, one may consider the various phases of sludge growth and BOD removal to consist of a dynamic relationship between the mass transfer of essential foods into the cell structure, and the assimilation and utilization of these foods for energy and growth. At high concentrations of organic matter, the rate of assimilation and the growth rate are independent of the concentration of organic matter. At low organic levels, the rate of growth and hence the rate of BOD removal are frequently concentration dependent. The kinetic form of Equation (2) describes the situation except during the endogenous phase.

Growth under the second and third phases is independent of the concentration of organics, x_1, since the organics are in excess, that is, $x_1 >> K$, and thus Equation (2) can be approximated by

$$\mu = k$$

During the initial part of the fourth phase of growth, μ is dependent on x_1 and the original form of Equation (2) applies, but as the organics are consumed, x_1, becomes small, that is, $x_1 << K$, and thus Equation (2) can be approximated by

$$\mu = \frac{kx_1}{K} \tag{4}$$

During the endogeneous phase, the effect of endogeneous respiration becomes important. In the expression for one phase kinetics employed by Grieves et al. (20), the effect of endogeneous respiration is considered. The expression is

$$r = \mu x_2 - k_D x_2$$

Substitution of Equation (2) in the above expression gives

$$r = \frac{kx_1 x_2}{K + x_1} - k_D x_2 \tag{5}$$

where

k_D = the specific endogeneous microbial attrition rate, hr^{-1}.

When $x_1 >> K$, Equation (5) becomes

$$r = kx_2 - k_D x_2 = (k - k_D)x_2 , \tag{6}$$

and when $x_1 << K$, Equation (5) becomes

$$r = \frac{kx_1 x_2}{K} - k_D x_2 \tag{7}$$

when

$$x_1 = \frac{k_D K}{k}$$

one has theoretically

$$r = o$$

Numerically k_D is usually two orders of magnitude less than k (20). Hence the effect of endogeneous respiration is negligible except when x_1 is very small (death phase). It should be pointed out that Equation (3) is no longer strictly valid if the death or endogeneous rate is included in the kinetic model as given by Equation (5). This is because of the definition of Y, that one milligram of organic is consumed to produce Y milligrams of organisms without considering any effect of the death rate constant. Hence, Equation (3) is not valid for the analysis if one uses Equation (5) as his model. However, one can still use the growth part of the kinetic model for organisms [the first part of Equation (5)] for the kinetics representing the rate of consumption of organic materials. Hence, using the definition of Y and using the growth part of the kinetic model, one can write

$$-r_s = \frac{k\ x_1\ x_2}{Y(K + x_1)} \tag{8}$$

This equation will be used as the kinetic model for representing the rate of consumption of organics and Equation (5) will be used as the kinetic model for representing the rate of production of organisms throughout this work.

2. THE MATHEMATICAL REPRESENTATION OF THE PROCESS

a. Flow Models

A plug flow model is often used to represent the flow behavior of the waste water treatment processes. This model assumes that there is no longitudinal mixing in the aeration tank. However, the optimum degree of longitudinal mixing in the aeration tank is still in question. McKinney (21) has advocated the use of aeration tanks designed to provide a uniform composition within the entire tank. The latter system is often referred to as the complete mixing waste water treatment process (21) and the completely mixed stirred tank model is usually used to represent the flow behavior in this system. In the subsequent discussion the completely mixed stirred tank model will be used.

b. Simplifying Assumptions

The following assumptions and simplifications are made in specifying the process and developing the mathematical representation for the process.

(1) The system is isothermal.

(2) Physical properties such as density, diffusivity, and viscosity are constant.

(3) Y is dependent only upon the property of the waste itself, and independent of the age of the organisms and the effect of other physical conditions such as the concentrations of organics and organisms.

(4) Organics and organisms are distinctly separate entities in solution.

(5) Sufficient oxygen is supplied for the oxidation.

(6) The fluid is a continuum and there is no segregation.

Some of these assumptions depart from reality, but they are justified on the grounds that they simplify the description of the process without appreciably changing its basic characteristics.

c. The Mathematical Representation

Based on the preceeding assumptions and the flow models described in the previous section one can visualize the system as consisting of reaction stages as shown in Figure 4. One also can define the following notations for subsequent analysis.

x_1^n = concentration of organics in the outlet stream of the nth stage, mg/liter,

x_1^0 = concentration of organics in feed, mg/liter,

x_2^n = concentration of organisms in the outlet stream of the nth stage, mg/liter,

x_2^0 = concentration of organisms in feed, mg/liter.

A reactor stage designated as the nth stage is shown in Figure 5. The essential governing equations are derived below.

i. Organism material balance. The quantity of organisms produced in each reactor can be expressed in terms of the quantity of organics consumed.

Accumulation = Input − Output + Production of organisms in the reactor.

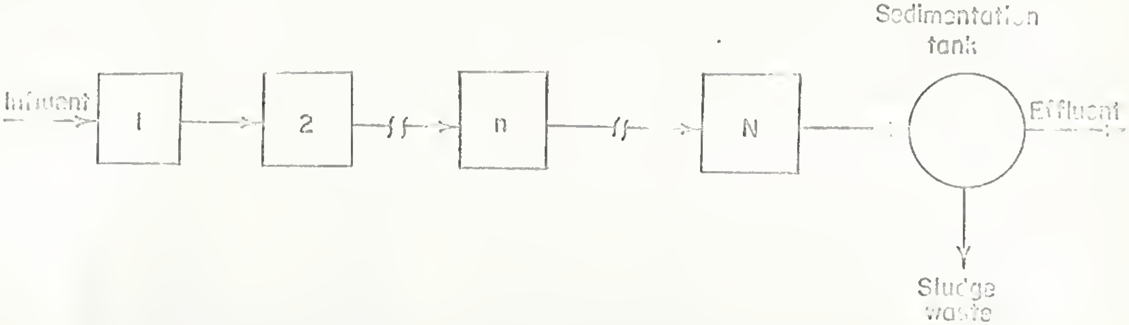


Fig. 4. N aeration tank model for waste treatment systems.

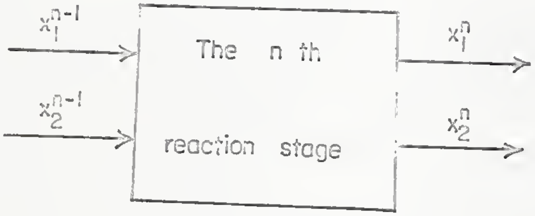


Fig. 5. A schematic representation of a reaction stage.

$$V^n \frac{dx_2^n}{dt} = qx_2^{n-1} - qx_2^n + V^n r^n \tag{9}$$

where

q = volumetric flow rate, liters/hr.

V^n = volume of the nth reactor, liters

r^n = rate of change of organism concentration due to growth, mg/liter, hr. [see Equation (5)]

$\frac{dx_2^n}{dt}$ = net rate of change of organism concentration in the reactor, as under transient condition, mg/liter, hr.

Here it is assumed that the volume of the reactor is the same as the volume of liquid in the reactor. It is also assumed that the volumetric flow rate remains constant throughout the process.

When Equation (9) is combined with an organism growth rate model [Equation (5)], it becomes, after simplification,

$$\frac{dx_2^n}{dt} = (x_2^{n-1} - x_2^n)\frac{1}{\bar{t}^n} + \frac{k\, x_1^n\, x_2^n}{K + x_1^n} - k_D\, x_2^n \tag{10}$$

where

$$\bar{t}^n = \frac{V^n}{q}$$

The $\bar{t}^n$ is called the nominal holding time or the normal retention time or the mean residence time for the nth reactor. It is the average length of time which particles in the feed remain in the vessel before being washed out. The actual residence times of individual particles very widely about $\bar{t}^n$, however.

ii. Organic material balance. Since the exit stream from the continuous flow stirred tank reactor has the same concentration of organics and organisms as the fluid within the reactor, one can write the material balance on organics as

$$V^n \frac{dx_1^n}{dt} = qx_1^{n-1} - qx_1^n + r_s^n V^n$$

where

r_s^n = rate of change of organic concentration due to its consumption, mg/liter, hr. [see Equation (8)]

$\frac{dx_1^n}{dt}$ = net rate of change of organic concentration in the reactor, as under transient condition, mg/liter, hr.

If one substitutes Equation (8) into the above expression and simplifies, then the organic material balance becomes

$$\frac{dx_1^n}{dt} = (x_1^{n-1} - x_1^n)\frac{1}{\bar{t}^n} - \frac{k\, x_1^n\, x_2^n}{Y(K + x_1^n)} \tag{11}$$

iii. Dimensional analysis. In order to make the results as general as possible, the performance equations [Equations (10) and (11)] are transferred into dimensionless form. The organic waste concentration x_1^n is made dimensionless by dividing by the steady state concentration of the organic waste in the influent, x_{1s}^0 (or x_{1s}^t). The organism concentration is made dimensionless by dividing by the product Yx_{1s}^0, thus

$$y_1^n = \frac{x_1^n}{x_{1s}^0} \quad , \qquad y_2^n = \frac{x_2^n}{Yx_{1s}^0}$$

where y_1^n is the dimensionless concentration of the organic waste in the nth aeration tank and y_2^n is the dimensionless organism concentration in the nth aeration tank. The constant K may also be made dimensionless by dividing it by x_{1s}^0, that is,

$$K_1 = \frac{K}{x_{1s}^0}$$

where K_1 is the dimensionless organic concentration at which the specific growth rate is one half the maximum value. The time, t, could have been made dimensionless by dividing it by the mean residence time in the nth reactor $\bar{t}^n$ or the overall mean residence time of the system $\bar{t}$

$$\theta = \frac{t}{\bar{t}^n}$$

where θ is the dimensionless time. Since all the simulation studies have been carried out on a desk top analog computer EAI TR-48 it is advisable to use the real time, t, instead of the dimensionless time, θ.

It is worth noting that the steady state influent organic concentration, x_{1s}^0, is x_1^0 as long as there is no disturbance in x_{1s}^0, that is, as long as x_{1s}^0 remains constant. It should also be noted that when x_{1s}^0 is equal to x_1^0 then all the dimensionless variables have a range from zero to one, since x_1^0 is the largest concentration in the system.

Now, organic and organism material balances, that is, Equations (11) and (10) respectively, can be rewritten using newly defined dimensionless variables as

$$\frac{dy_1^n}{dt} = (y_1^{n-1} - y_1^n)\,\frac{1}{\bar{t}^n} - \frac{k\,y_1^n\,y_2^n}{K_1 + y_1^n} \qquad (12)$$

and

$$\frac{dy_1^n}{dt} = (y_2^{n-1} - y_2^n)\,\frac{1}{\bar{t}^n} + \frac{k\,y_1^n\,y_2^n}{K_1 + y_1^n} - k_D\,y_2^n \qquad (13)$$

respectively. Equations (12) and (13) have the units of resiprocal time and they can be rewritten as

$$\frac{dy_1^n}{dt} = (y_1^{n-1} - y_1^n)\,\frac{1}{\bar{t}^n} - \frac{\tau^n}{\bar{t}^n}\left(\frac{y_1^n\,y_2^n}{K_1 + y_1^n}\right) \qquad (14)$$

and

$$\frac{dy_2^n}{dt} = (y_2^{n-1} - y_2^n)\,\frac{1}{\bar{t}^n} + \frac{\tau^n}{\bar{t}^n}\,\frac{y_1^n\,y_2^n}{K_1+y_1^n} - K_2\,y_2^n \qquad (15)$$

respectively, and where τ^n is the dimensionless mean holding time or the dimensionless mean residence time and K_2 is the dimensionless endogeneous respiration rate. They are defined as

$$\tau^n = k\,\bar{t}^n$$

$$K_2 = \frac{k_D}{k}$$

CHAPTER III

ANALSES OF STEADY STATE AND CRITICAL CONDITIONS

1. ANALYSIS OF STEADY STATE

At the steady state there is neither change in organic concentration nor in the organism concentration with time, that is, in the transient equations of the system [Equations (14) and (15)]

$$\frac{dy_1^n}{dt} = 0 \qquad \text{and} \qquad \frac{dy_2^n}{dt} = 0$$

Thus, the steady state performance equations of the system are

$$y_1^{n-1} - y_1^n - \frac{\tau^n \, y_1^n \, y_2^n}{K_1 + y_1^n} = 0 \tag{16}$$

and

$$y_2^{n-1} - y_2^n + \tau^n \left[\frac{y_1^n \, y_2^n}{K_1 + y_1^n} - K_2 \, y_2^n\right] = 0 \tag{17}$$

It is assumed in the remaining part of this work that the feed is sterile; that is, there are no organisms in the influent stream ($y_2^f = y_2^0 = 0$). Therefore, an obvious solution of the steady-state equations is given by $y_{1s}^n = y_{1s}^{n-1} = \ldots = y_{1s}^0 = 1$ and $y_{2s}^n = y_{2s}^{n-1} = \ldots = y_{2s}^0 = 0$, where y_{1s}^n and y_{2s}^n, $n = 0, 1, \ldots, n$, represent the steady-state organic and organism concentrations respectively. This represents the so-called washout condition (24, 26), and this steady state may be referred to as the washout steady-state. Thus, when the washout steady-state is "stable," the continuous waste water treatment process will not reduce the organic content of waste by growing the organisms, and the system will always be filled with a sterile (no organisms in the feed, i.e. $y_2^f = y_2^0 = 0$) medium having the influent organic concentration. The minimum mean holding time (maximum dilution rate) is that below which washout occurs. This mean holding time can be evaluated analytically or numerically by examining Equations (16) and (17) around critical or limiting conditions of operation or by the method of stability analysis (24).

The algebraic expressions of steady-state [Equations (16) and (17)] predict another steady-state which is not the washout steady state. This steady state will be referred to as the normal steady state since it represents the condition of normal operation. From Equation (16), one has

$$\frac{\tau^n y_1^n y_2^n}{K_1 + y_1^n} = y_1^{n-1} - y_1^n$$

and substitution of the above expression into Equation (17) gives

$$y_2^{n-1} - y_2^n + y_1^{n-1} - y_1^n - \tau^n K_2 y_2^n = 0$$

Solving the above expression for y_1^n and y_2^n yields

$$y_1^n = y_1^{n-1} + y_2^{n-1} - (1 + \tau^n K_2) y_2^n \tag{18}$$

and

$$y_2^n = \frac{y_1^{n-1} + y_2^{n-1} - y_1^n}{1 + \tau^n K_2} \tag{19}$$

respectively. Substitution of Equation (19) into Equation (16) yields

$$y_1^{n-1} - y_1^n - \frac{\tau^n\ y_1^n}{K\ + y_1^n}\ [\frac{y_1^{n-1} + y_2^{n-1} - y_1^n}{1 + \tau^n\ K_2}] = 0$$

Simplification and rearrangement of the above expression gives

$$[1 + \tau^n(K_2 - 1)](y_1^n)^2 + [(K_1K_2 - K_2\ y_1^{n-1} + y_1^{n-1} + y_2^{n-1})\tau^n$$

$$+ [- (1 + \tau^n\ K_2)K_1y_1^{n-1}] = 0 \tag{20}$$

The solution of this quadratic equation is

$$y_1^n = \frac{- b \pm \sqrt{(b^2 - 4ac)}}{2a} \tag{21}$$

where

$$a = 1 + \tau^n(K_2 - 1) \tag{22}$$

$$b = [(K_1K_2 - K_2\ y_1^{n-1} + y_1^{n-1} + y_2^{n-1})\tau^n + K_1 - y_1^{n-1}] \tag{23}$$

$$c = - (1 + \tau^n\ K_2)K_1\ y_1^{n-1} \tag{24}$$

Equation (23) can be rewritten as

$$b = (K_1K_2 + y_2^{n-1})\tau^n - [1 + (K_2 - 1)\tau^n]y_1^{n-1} + K_1$$

or

$$b = (K_1K_2 + y_2^{n-1})\tau^n + K_1 - a\ y_1^{n-1} \tag{25}$$

Since y_1^{n-1}, K_1, K_2, and τ^n are all non-negative numbers, c will always be a non-positive number. Hence equation (21) can be rewritten, using this fact, as

$$y_1^n = \frac{-\ b \pm \sqrt{(b^2 - 4a(-|c|))}}{2a} \tag{26}$$

It can be seen that there are two values of y_1^n, which satisfy Equation (26). If both values of y_1^n are in the range $0 \leq y_1^n \leq 1$, there are two steady state conditions. However, if only one of the y_1^n's is in this range, there is only one steady state condition. The following discussion shows how one can determine the proper sign before the radical in Equation (26) in order to obtain a feasible solution or solutions satisfying the conditions of $0 \leq y^n \leq 1$.

Case I. $a > 0$. It can be seen from Equation (22) that when $a > 0$, one has

$$1 + \tau^n(K_2 - 1) > 0$$

or

$$\tau^n < \frac{1}{1 - K_2} = \tau_{am}^n = k\bar{t}_{am}^n \tag{27}$$

where $\bar{t}_{am}^n$ is the minimum mean holding time corresponding to the condition where the organic and organism concentrations approach assymptotically to ∞ and − ∞ respectively, that is, the condition where $y_1^n \to \infty$ and $y_2^n \to -\infty$. $\bar{t}_{am}^n$ is discussed further in the next section. Since a > 0, Equation (26) can be rewritten as

$$y_1^n = \frac{-b \pm \sqrt{b^2 + 4|a||c|}}{2|a|} \tag{28}$$

Since

$$\sqrt{b^2 + 4|a||c|} > b,$$

one must choose a positive sign before the radical in Equation (28) to have $y_1^n \geq 0$. If one chooses, instead, the negative sign before the radical in Equation (28), one has $y_1^n < 0$, which is not feasible. Thus, there is only one steady-state solution for the case a > 0 and this steady-state solution should be the washout steady-state if the feed is sterile; that is, the condition given by $y_{1s}^n = y_{1s}^{n-1} = \ldots = y_{1s}^0 = 1$ and $y_{2s}^n = y_{2s}^{n-1} = \ldots = y_{2s}^0 = 0$. This can also be varified numerically as follows.

Equations (22), (23), and (24) can be simplified for the steady-state washout condition as

$$a = 1 + \tau^n (K_2 - 1)$$
$$b = (K_1K_2 - K_2 + 1)\ \tau^n + (K_1 - 1)$$
$$c = -(1 + K_2\ \tau^n)K_1$$

respectively. The above expression for 'b' can be rearranged to give

$$b = -(a + c)$$

Because $a > 0$ and $c < 0$, one has

$$b = -(|a| - |c|)$$

Hence, the right hand side of Equation (28) gives a value of one for the steady-state washout condition as follows, if the positive sign before the radical is chosen. This is shown below

$$\text{R.H.S.} = \frac{(|a| - |c|) + \sqrt{[-(|a| - |c|)]^2 + 4|a|\ |c|}}{2\ |a|}$$

$$= \frac{|a| - |c| + \sqrt{(|a| + |c|)^2}}{2\ |a|}$$

$$= \frac{|a| - |c| + |a| + |c|}{2\ |a|}$$

$$= 1$$

The left hand side of Equation (28) is equal to one for the washout condition. Hence the required identity has been proved numerically. Similarly, for the steady state washout condition one can obtain the identity form Equation (19) as

$$0 = 0$$

Case II. $a < 0$. It can be seen from Equation (22) that when $a < 0$, one has

$$1 + \tau^n (K_2 - 1) < 0$$

or

$$\tau^n > \frac{1}{1 - K_2} = \tau^n_{am} = k\bar{t}^n_{am}$$

Since, a < 0, Equation (25) implies that one must have b > 0. Equation (26) can then be rewritten as

$$y_1^n = \frac{-|b| \pm \sqrt{[|b|^2 - 4(-|a|)(-|c|)]}}{2(-|a|)} \qquad (29)$$

Since

$$\sqrt{[|b|^2 - 4(-|a|)(-|c|)} < |b| ,$$

one can choose any of the two signs in Equation (29) to have $y_1^n \geq 0$. Hence there might be two steady state solutions for the case a < 0.

First consider that the negative sign before the radical in the Equation (29) is chosen.

This gives

$$y_1^n = \frac{|b| + \sqrt{[|b|^2 - 4(-|a|)(-|c|)]}}{2|a|}$$

Since

$$0 \leq y_1^n \leq 1,$$

one can see

$$0 \leq |b| + \sqrt{(|b|^2 - 4(-|a|)(-|c|))} \leq 2|a|$$

or

$$|b| \leq 2|a|$$

Because a < 0 and b > 0, one must have

$$b + 2a \leq 0$$

Substituting the value of 'a' from Equation (22) and that of 'b' from Equation (25) into the above expression and simplifying the resulting expression gives

$$\tau^n \leq \frac{1 + K_1}{1 - K_2(1 + K_1)} = \tau^n_{wm} = k\ \bar{t}^n_{wm} \qquad (30)$$

where $\bar{t}^n_{wm}$ is the minimum mean holding time corresponding to the washout condition which will be elaborated in the next section. It has already been shown that one must have

$$\tau^n > \frac{1}{1 - K_2} = \tau^n_{am} = k\ \bar{t}^n_{am}$$

for 'a' to be negative. Therefore, a steady-state solution can be obtained when the negative sign before the radical in Equation (29) is chosen as long as the condition given by Equation (30) and the expression given above are simultaneously satisfied. These two conditions can be combined to give

$$k\,\bar{t}^{n}_{am} = \frac{1}{1 - K_2} < \tau^{n} \leq \frac{1 + K_1}{1 - K_2(1 + K_1)} = k\,\bar{t}^{n}_{wm} \qquad (31)$$

This steady state solution is the washout steady state solution. This means that one has the condition of $y^{n}_{1s} = y^{n-1}_{1s} = \ldots = y^{0}_{1s} = 1$ and $y^{n}_{2s} = y^{n-1}_{2s} = \ldots = y^{0}_{2s} = 0$. This can also be varified numerically as done in the case of $a > 0$.

In the previous case of $a > 0$, it is shown that for the washout steady state condition, one has

$$b = -\,(a + c)$$

Now, because $a < 0$ and $c < 0$, one has

$$b = -\,[(-|a|) + (-|c|)]$$

or

$$|b| = |a| + |c|$$

Hence, the right hand side of Equation (29) can be rewritten for the steady-state washout condition by choosing the negative sign before the radical sign as

$$\text{R.H.S.} = \frac{-[|a| + |c|] - \sqrt{[|a| + |c|]^2 - 4(-|a|)(-|c|)}}{2(-\,|a|)}$$

$$= \frac{|a| + |c| + \sqrt{[|a| - |c|]^2}}{2\,|a|}$$

$$= \frac{|a| + |c| + |a| - |c|}{2|a|}$$

$$= 1$$

The left hand side of the Equation (29) is always one for the washout condition. Hence, the necessary equality of Equation (29) is satisfied. Similarly, for the steady state washout condition one can show the left hand side of the Equation (19) is equal to the right hand side of the same equation which are both zero.

Now, consider the second possibility of having $y_1^n \geq 0$; that is, consider the positive sign before the radical in Equation (29). This gives

$$y_1^n = \frac{-|b| + \sqrt{[|b|^2 - 4(-|a|)(-|c|)]}}{2(-|a|)}$$

or

$$y_1^n = \frac{|b| - \sqrt{[|b|^2 - 4(-|a|)(-|c|)]}}{2\,|a|}$$

Since

$$0 \leq y_1^n \leq 1,$$

one can see that

$$0 \leq |b| - \sqrt{[|b|^2 - 4(-|a|)(-|c|)} \leq 2|a|$$

or

$$|b| \overset{\leq}{\underset{>}{=}} 2|a|$$

Because a < 0 and b > 0, one must have

$$b + 2a \overset{>}{\underset{<}{=}} 0$$

Substituting the value of 'a' from Equation (22) and that of 'b' from Equation (25) into the above expression and simplifying the resulting expression gives

$$\tau^n \overset{<}{\underset{>}{=}} \frac{1 + K_1}{1 - K_2\ (1 + K_1)} = \tau^n_{am} = k\ \bar{t}^n_{wm}$$

It has already been shown that one must have

$$\tau^n > \frac{1}{1 - K_2} = \tau^n_{am} = k\ \bar{t}^n_{am}$$

for 'a' to be negative. These expressions can be combined to give

$$k\ \bar{t}^n_{am} < \tau^n \overset{<}{\underset{>}{=}} \frac{1 + K_1}{1 - K_2(1 + K_1)} = k\ \bar{t}^n_{wm} \tag{32}$$

Therefore, a steady-state solution can be obtained when the positive sign before the radical in Equation (29) is chosen as long as the condition given by Equation (32) is satisfied. Strictly speaking equation (32) must be written as

$$k\,\bar{t}_{am} < \tau^n \le \frac{1 + K_1}{1 - K_2(1 + K_1)} = k\,\bar{t}^{n}_{wm}$$

and

$$\tau^n > \frac{1 + K_1}{1 - K_2(1 + K_1)} = \tau_{wm} = k\,\bar{t}_{wm} > k\,\bar{t}_{am}$$

The first expression is the same as Equation (31) and therefore a washout steady state is realized, as shown before, as long as the first expression is satisfied. If the second expression is satisfied, there is obviously a steady state solution which is the normal steady state solution [note that $\tau^n > \tau_{wm}$].

It is worth noting that as long as Equation (31) is satisfied, there are two steady state solutions which are obtained by choosing respectively the positive and negative signs before the radical in Equation (29). As stated previously and also shown numerically, both of the steady-state solutions are the washout steady-state solutions, but it might be possible that one of them is stable and the other unstable.

It can be seen that Equation (21) is in a form which is convenient for an iterative computation on the digital computer. However, the use of this equation involves a cumbersome procedure for determining the sign before the radical involved in the equation as discussed above. There is a simpler procedure than the use of Equation (21) which gives a unique feasible solution of y_1^n (17). First, Equation (16) is solved for τ^n to obtain

$$\tau^n = \frac{(y_1^{n-1} - y_1^n)(K_1 + y_1^n)}{y_1^n \, y_2^n} \tag{33}$$

Substituting this result into Equation (16) gives

$$y_2^n = y_2^{n-1} + \frac{(y_1^{n-1} - y_1^n)[y_1^n - K_2(K_1 + y_1^n)]}{y_1^n} \tag{34}$$

Now, assuming a value of y_1^n, y_2^n can be calculated uniquely from Equation (34). Once y_2^n is known, τ^n can be determined uniquely from Equation (33). Note that as long as x_1^0 remains constant at x_1^0, y_1^n and y_2^n are values between zero and one.

2. MINIMUM MEAN HOLDING TIMES FOR WASHOUT CONDITION

As noted in the preceding section, the condition of $y_{1s}^n = y_{1s}^{n-1} = \ldots = y_{1s}^0 = 1$ and $y_{2s}^n = y_{2s}^{n-1} = \ldots = y_{2s}^0 = 0$, represents the condition of washout, and the steady state corresponding to this condition may be referred to as the washout steady state. By "washout" one means the condition under which the influent flow rate of sterile waste is so high that there is no opportunity for organisms to remain in the system to function. Under the washout steady state, therefore, the waste water treatment process does not reduce the organic content of waste by growing organisms and the system is always filled with sterile medium having the influent organic concentration.

The minimum mean holding time for an individual reactor, corresponding to this washout condition and denoted by $\bar{t}_{wm}^n$ can be determined as follows;

$$\tau^{n}_{wm} = k\,\bar{t}^{n}_{wm} = \lim_{\substack{y_1^n \rightarrow y_1^{n-1},\ y_1^{n-1} \rightarrow y_1^{n-2},\ \ldots,\ y_1^1 \rightarrow y_1^0 = 1 \\ y_2^n \rightarrow y_2^{n-1},\ y_2^{n-1} \rightarrow y_2^{n-2},\ \ldots,\ y_2^1 \rightarrow y_2^0 = 0}} \tau^{n}$$

$$= \lim_{\substack{y_1^n \rightarrow 1,\ y_1^{n-1} \rightarrow 1 \\ y_2^n \rightarrow 0,\ y_2^{n-1} \rightarrow 0}} \frac{(y_1^{n-1} - y_1^n)(K_1 + y_1^n)}{y_1^n\, y_2^n}$$

$$= \lim_{\substack{y_1^n \rightarrow 1,\ y_1^{n-1} \rightarrow 1 \\ y_2^n \rightarrow 0,\ y_2^{n-1} \rightarrow 0}} \left(\frac{y_1^{n-1} - y_1^n}{y_2^n}\right) \lim_{\substack{y_1^n \rightarrow 1 \\ y_2^n \rightarrow 0}} \left(\frac{K_1 + y_1^n}{y_1^n}\right)$$

$$= \lim_{\substack{y_1^n \rightarrow 1,\ y_1^{n-1} \rightarrow 1 \\ y_2^n \rightarrow 0,\ y_2^{n-1} \rightarrow 0}} \frac{\dfrac{d}{dy_1^n}(y_1^{n-1} - y_1^n)}{\dfrac{d}{dy_1^n}(y_2^n)} \lim_{y_1^n \rightarrow 1} \frac{K_1 + y_1^n}{y_1^n}$$

Since

$$\lim_{y_1^n \rightarrow 1,\ y_1^{n-1} \rightarrow 1} \frac{d}{dy_1^n}(y_1^{n-1} - y_1^n) = \lim_{y_1^n \rightarrow 1} \frac{d}{dy_1^n}(1 - y_1^n) = 1$$

and, from Equation (34),

$$\lim_{\substack{y_1^n \to 1,\ y_2^{n-1} \to 1 \\ y_2^n \to 0,\ y_2^{n-1} \to 0}} \frac{d}{dy_1^n}(y_2^n) = [1 - K_2(1 + K_1)],$$

one obtains

$$\tau_{wm}^n = k\,\bar{t}_{wm}^n = \frac{K_1 + 1}{1 - K_2(k + K_1)} \qquad (35)$$

or

$$\bar{t}_{wm}^n = \frac{K_1 + 1}{k[1 - K_2(1 + K_1)]} \qquad (36)$$

Thus, when $\bar{t}^n \leq \bar{t}_{wm}^n$ washout occurs and when $\bar{t}^n > \bar{t}_{wm}^n$ a normal steady-state operation can be maintained.

$\bar{t}_{wm}^n$ can also be obtained when the stability of the system is analyzed by the method of stability analysis based on the principle that the local stability of any steady state is assured when all the eigenvalues of the stability matrix (obtained by linearizing the differential equations, Equations (16) and (17), about the pertinent steady state) have negative parts. Tsuchiya et al. (25) and Ramkrishna et al. (26) have derived an expression similar to Equation (36) using this approach for a continuous one stage system and neglecting the endogeneous respiration term. In general, the following observations about a system consisting of completely stirred reactors connected in series and operated under the steady state condition are noted below.

(1) There will never be a washout condition in the system with a non-sterile feed since the organisms are continuously fed into the system and they consume organics in the feed continuously by reproducing more organisms, regardless of the sizes of reactors in the system. In other words, the washout condition can occur only when the system is operated with the sterile feed ($y_2^f - y_2^0 = 0$).

(2) If the first reactor is not under the washout condition there will never be a washout condition in any of the succeeding reactors since the feed to the subsequent reactors will not be a sterile feed.

(3) If any of the reactors is under the condition of stable washout every other reactor following it will be under the condition of stable washout as long as its size is the same as or smaller than the first reactor. It is also noted that washout in the subsequent reactors can be prevented if and only if the size of these reactors is increased as compared to the first reactor under the condition of washout.

Now, for the condition at which y_1^n approaches infinity and y_2^n approaches minus infinity, there must be a corresponding minimum dimensionless mean holding time which will be denoted by τ_{am}^n or $k\ \bar{t}_{am}^n$. This is an asymptotic minimum mean holding time and y_1^n and y_2^n will approach asymptotically to a vertical axis passing through τ_{am}^n or $k\ \bar{t}_{am}^n$.

It can be seen from Equation (21) that if a = 0 then y_1^n will be infinity and therefore, from Equation (19), y_2^n will be minus infinity. In other words, for this asymptotic washout condition, one must have a = 0 where 'a' is given by Equation (22), that is,

$$a = 1 + \tau^n(K_2 - 1) = 0$$

Solving the above expression for τ^n yields

$$\tau^n_{am} = k\,\bar{t}^n_{am} = \frac{1}{1 - K_2} \qquad (37)$$

or

$$\bar{t}^n_{am} = \frac{1}{k(1 - K_2)} \qquad (38)$$

It is worth noting that when $K_1 = 0$ in the Equation (36), it reduces to Equation (38), that is, one has

$$\bar{t}^n_{wm} = \bar{t}^n_{am}$$

3. EXTREME VALUES OF ENDOGENEOUS RESPIRATION CONSTANT

The theoretically lowest possible value of endogeneous respiration constant, k_D, is apparently zero. This corresponds to the situation in which the organism grows at all times without any accompanying death process due to endogeneous respiration.

The theoretically highest value of k_D will be that corresponding to the situation where organisms die as soon as they are produced, that is, the growth and death process occur simultaneously at the same rate. The above situation is equivalent to saying that $r = 0$ for the batch process, where r is given by Equation (5). Hence,

$$r = \frac{k\ x_1\ x_2}{K + x_1} - k_D\ x_2 = 0$$

Solving the above expression for k_D gives

$$k_D = \frac{k\ x_1}{K+x_1}$$

or

$$k_D = \frac{k}{\frac{K}{x_1} + 1}$$

Now, k_D is largest when x_1 is also largest, that is, when x_1 is equal to $x_1(0)$. Hence

$$(k_D)_{max} = \frac{k}{\frac{K}{x_1(0)} + 1} \qquad (39)$$

It can be seen from the above equation that for a given value of k_D, one has

$$k_D \leq \frac{k}{\frac{K}{x_1(0)} + 1}$$

The simplification of the above expression gives

$$x_1(0) \leq \frac{1 - K_2}{K_2 K}$$

In other words, for any batch culture, one should have the initial organic nutrient concentration at least as large as that given by the right hand side of the above expression for the organixms to have a chance to survive.

A similar analysis is applied to the flow reactor (continuous culture) to obtain a expression of $(k_D)_{max}$. The highest value of k_D will be that corresponding to the situation where organisms die as soon as they are produced, as mentioned previously. This situation is equivalent to saying that

$$\tau^n \left(\frac{y_1^n \, y_2^n}{K_1 + y_1^n} - K_2 \, y_2^n\right) = 0$$

in the steady state flow reactor equation [Equation (17)]. The above expression is equivalent to the $r = 0$ in the batch reactor. The above expression gives

$$\frac{y_1^n}{K_1 + y_1^n} - K_2 = 0 \quad \text{and} \quad y_2^n = 0$$

The first expression gives

$$K_2 = \frac{y_1^n}{K_1 + y_1^n}$$

Under the condition being considered (zero rate of transformation due to the reaction) apparently one has $y_2^n = 0$ and $y_1^n = 1$ which is the maximum value of y_1^n. Therefore,

$$(K_2)_{max} = \frac{1}{1 + K_1} \tag{40}$$

or

$$(k_D)_{max} = \frac{k}{\frac{K}{x_{1s}^0} + 1} \tag{41}$$

Equation (41) for the flow reactor is very similar to Equation (39) for the batch reactor. It can be seen from Equation (41) that for a given value of k_D, one has to have

$$x_{1s}^0 \geq \frac{1 - K_2}{K_2 K}$$

This means that one should feed the influent with an organic concentration at least as large as that given by the right hand side of the above expression for the organisms to have a chance to survive in a system consisting of completely mixed flow reactions (continuous culture).

4. A SYSTEM WITH A SINGLE COMPLETELY MIXED FLOW REACTOR

In order to obtain a better understanding of the results of the analyses of the steady-state and critical conditions of the system, a system with a single completely mixed flow reactor is considered. The following values are assumed for some of the constants and parameters in this work.

$k = 0.1$, hr^{-1}

$k_D = 0.002$, hr^{-1}

$K_2 = \frac{k_D}{k} = 0.09$, dimensionless

$K_1 = 0.1$, dimensionless

$Y = 0.5$, mg/mg,

The maximum permissible value of the dimensionless endogeneous respiration rate, K_2 and in turn the maximum permissible value of k_D are estimated by using Equations (40) and (41) as shown below.

$$(K_2)_{max} = 0.91, \text{ dimensionless}$$

or

$$(k_D)_{max} = 0.091, \text{ hr}^{-1}.$$

The value of k_D employed here is definitely smaller than this permissible maximum limit. The minimum mean holding time corresponding to washout steady-state, $\bar{t}^n_{wm}$, and the minimum asymptotic mean holding time for the condition $y^n_1 \to \infty$ and $y^n_2 \to -\infty$, $\bar{t}^n_{am}$ are calculated for the system under consideration using Equations (36) and (38) respectively. The results are

$$\bar{t}_{wm} = 11.02, \text{ hr}$$

and

$$\bar{t}_{Am} = 10.02, \text{ hr}$$

Table I has been prepared by assuming different values of y^1_1 in Equation (34) and calculating the values of y^1_2 and τ^1 using Equations (34) and (33) respectively. Figure 6 has been prepared based on Table I. Here the dimensionless organic and organism concentrations are

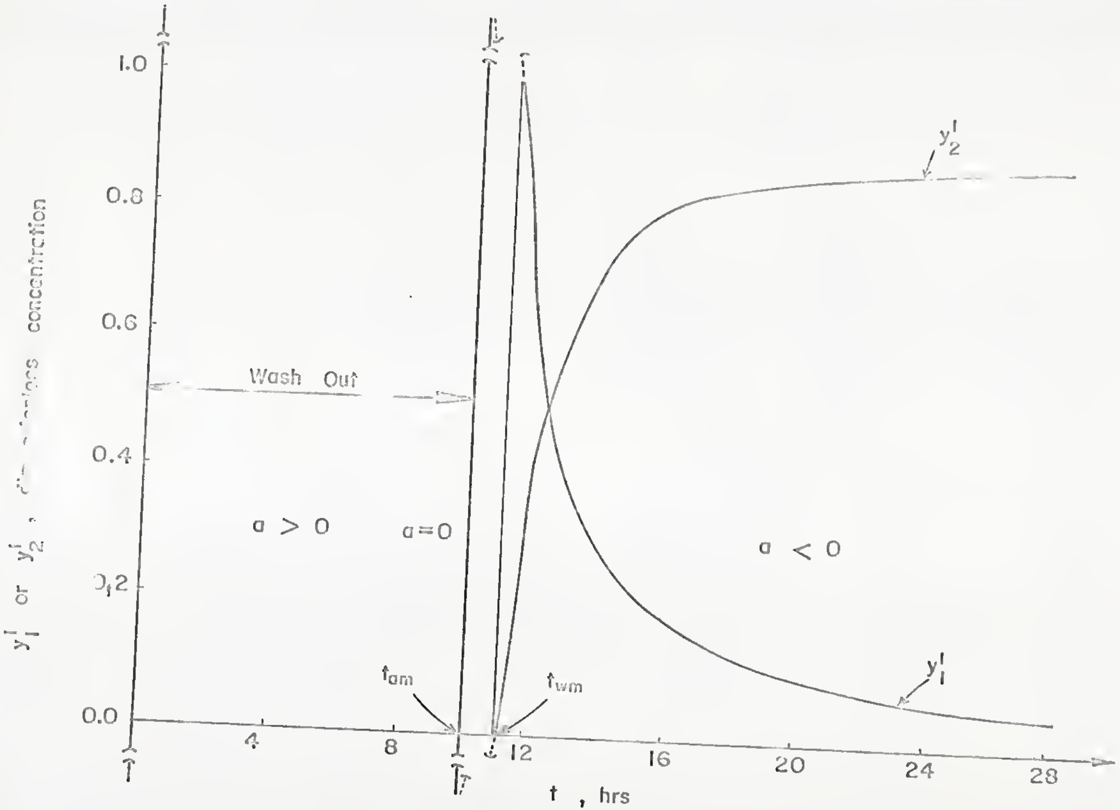


Fig. 6. y_1' or y_2 vs t with $\bar{t}_{am}$ and $\bar{t}_{wm}$.

Table I

Steady-state values of y_1^1 and y_2^1 for corresponding mean holding time of a single completely mixed flow reactor system

y_1^1	y_2^1	τ^1	$\bar{t}^1$, hr
∞	$-\infty$	1.002	10.02
1.0	0.0000	1.102	11.02
0.9	0.0978	1.136	11.36
0.8	0.1952	1.151	11.51
0.7	0.2930	1.170	11.70
0.6	0.3910	1.190	11.90
0.5	0.4880	1.230	12.30
0.4	0.5850	1.280	12.80
0.3	0.6810	1.368	13.68
0.2	0.7750	1.550	15.50
0.1	0.8640	2.084	20.84
0.09	0.8720	2.210	22.10

plotted against the mean holding time of the system. The two vertical axes are also drawn, which pass through $\bar{t}_{am}$ and $\bar{t}_{wm}$.

Chapter IV

DYNAMIC ANALYSIS OF THE WASTE WATER TREATMENT PROCESS

1. INTRODUCTION

Many studies, both theoretical and experimental, have been carried out to investigate the steady state characteristics of the continuous waste water treatment process. However, relatively few studies have been undertaken to study the dynamic characteristics of the system. Dynamic analysis has been a great aid to chemical engineers in gaining understanding of chemical processes. It seems logical that the same techniques will be of considerable assistance to biochemical engineers in gaining insight into biological processes.

Essential to dynamic analysis is the concept of a signal (31). Dynamic analysis is performed by measuring the time relationships between input and output signals. Some of the useful input variations are step, pulse, ramp, periodic, and random inputs. A step change is an instantaneous shift from one intensity of input to another. A periodic input such as a sine wave repeats at a fixed period of time.

The present chapter deals with the dynamic response of the continuous biological waste-water treatment system. The transient condition of the system is observed by plotting the system variables against time. The transient condition of the system is also observed by use of a phase-plane plot, since the mathematical models [Equations (5) and (8)] are described in terms of two dependent (state) variables. In this work, the temperature, aeration rate, and mixing condition are assumed to remain constant, and specifically a system consisting of a single completely mixed flow reactor is considered.

To carry out the computation it is necessary to assume values for some of the constants and parameters. Values of K reported by Washington, Hetling and Rao (28) for different organic concentrations range from 2 to 40 mg/liter. Since the concentration of the influent entering a waste treatment system is usually between about 100 and 1000 mg/liter, the values of K_1 should usually be between about 0.002 and 1.0. The following values are used in this investigation.

$k = 0.1$, hr^{-1}

$k_D = 0.002$, hr^{-1}

$K_2 = \frac{k_D}{k} = 0.02$, dimensionless

$K = 20$, mg/liter

$x_{1s}^0 = 200$, mg/liter

$K_1 = \frac{K}{x_{1s}^0} = 0.1$, dimensionless

$x_{2s}^0 = 0$ mg/liter

$Y = 0.5$, mg/mg

$V = 1000$, liters

2. TRANSIENT RESPONSE OF THE SYSTEM TO AN INPUT OF A CONSTANT INFLUENT ORGANIC CONCENTRATION AND A CONSTANT FLOW RATE

a. Performance Equations

As mentioned in the preceding section, a system consisting of a single completely mixed flow reactor is considered. For this system, the general organic and organism material balances [Equations (14) and (15)] reduce to

$$\frac{dy_1}{dt} = (y_1^0 - y_1)\frac{1}{t} - \frac{\tau}{t}\left(\frac{y_1\, y_2}{K_1 + y_1}\right) \qquad (42)$$

and

$$\frac{dy_2}{dt} = (y_2^0 - y_2)\frac{1}{t} + \frac{\tau}{t}\left(\frac{y_1\, y_2}{K_1 + y_1} - K_2\, y_2\right) \qquad (43)$$

respectively. Since the system consists of only one stage, the superscript 1 representing the stage number is omitted in the above equations and also in the subsequent discussions. It is also assumed in this section that after operation of the process is initiated (or feed conditions are changed to new conditions) the influent organic concentration, x_1^0, and the influent flow rate, q, are maintained at constant values* of x_{1s}^0 and q_s respectively.

b. Scaling and Static Test for the Analog Computer

The magnitude scaling for the system variables is summarized in Table II.

The scaled equation can now be written by substituting the computer variables from Table II into the original system equations [Equations

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*If one considers the start-up or restart-up problem then x_{1s}^0 and q_s are the values corresponding to the same steady state of that plant which it obtains after the operation. On the other hand if one considers the disturbances in q and x_1^0 then q_s and x_{1s}^0 are the values before the disturbances have occurred.

(42) and (43)]. This gives

$$\frac{d[\frac{y_1}{2}]}{dt} = (\frac{1}{2\beta\bar{t}})\, y_1^0 - (\frac{1}{\beta\bar{t}})[\frac{y_1}{2}] - (\frac{\tau}{\beta\bar{t}})\, \frac{[\frac{y_1}{2}][\frac{y_2}{2}]}{[\frac{K_1+y_1}{2}]} \tag{44}$$

and

$$\frac{d[\frac{y_2}{2}]}{dt} = (\frac{1}{2\beta\bar{t}})\, y_2^0 - (\frac{1}{\beta\bar{t}})[\frac{y_2}{2}] + (\frac{\tau}{\beta\bar{t}})\, \frac{[\frac{y_1}{2}][\frac{y_2}{2}]}{[\frac{K_1+y_1}{2}]} - (\frac{K_2\tau}{\beta t})[\frac{y_2}{2}] \tag{45}$$

respectively. In the above equations β is a time-scale factor. Because the influent organic concentration is assumed to remain constant for this problem, x_1^0 is always equal to x_{1s}^0. Hence the value of y_1^0 equal to one since y_1 is defined as the ratio of x_1 to x_{1s}^0. The value of y_2^0 is equal to zero since x_2^0 is maintained at zero. The other values of the parameters and constants are given in the preceding section.

The scaled analog diagram for the analog computation is shown in Figure 7. The pot settings for the static test and for the actual run are shown in Table III. The output voltages for each pot and each amplifier for the static test are also shown in Tables III and IV respectively.

c. Results and Discussion

The dimensionless organic concentration, y_1, and dimensionless organism concentration, y_2, are plotted in Figure 8 against time with the flow rate of zero liters/hr. Since the flow rate is zero liters/hr., these response curves in Figure 8 represent the batch kinetics. It is

Table II

Magnitude Scaling Summary of System Variables for Section 2 of Chapter 4

Problem Variable	Expected Maximum Value	Computer Variable
y_1	2*	$[\frac{y_1}{2}]$
y_2	2	$[\frac{y_2}{2}]$
$K_1 + y_1$	2	$[\frac{K_1 + y_1}{2}]$
$\frac{y_1}{K_1 + y_1}$	1	$[\frac{y_1}{2}]/[\frac{K_1 + y_1}{2}]$
$\frac{y_1\ y_2}{K_1 + y_1}$	2	$[\frac{[\frac{y_1}{2}]\ [\frac{y_2}{2}]}{[\frac{K_1+y_1}{2}]}]$

*The expected maximum value of y_1 is 1, but for simplicity and for maintaining symmetry with y_2, 2 was used.

noted in this figure that organisms grow rapidly in the beginning until they use up all of the organic materials in the system and then start dying slowly. In other words, the exponential phase of growth comes to an end when the organics are exhausted. It takes an infinitely long time (exponential decay) for all the organisms to die in a batch system.

Transient responses of the system to a constant influent organic concentration and to an influent flow rate after the onset of plant operation are plotted in Figures 9 and 10 with the influent flow rate as parameter. The initial condition of organism concentration, $y_2(0)$, is 0.0012, and this condition is probably equivalent to an innoculation of the system by a small quantity of bacteria at the start-up of the plant. It has been observed that there are very small changes or almost no changes in transient curves even when $y_2(0)$ is varied from 0.004 to 0.0016. The initial condition of organic concentration, $y_1(0)$, is 1 for this work. The system under this initial concentration can also be considered as originally being operated under the steady state condition with the flow rate near the washout condition, where $y_1 = 1^-$ and $y_2 = 0^+$. Therefore, the transient curves in Figures 9 and 10 can also be considered as the responses of the system to a step change in the flow rate from this near washout flow rate to new flow rates appearing as a parameter. That is, these figures show how the systam will reach its new steady state value after introducing a step change in the flow rate.

It can be seen from Figure 10 that $q = 90^+$ liters/hr., is indeed

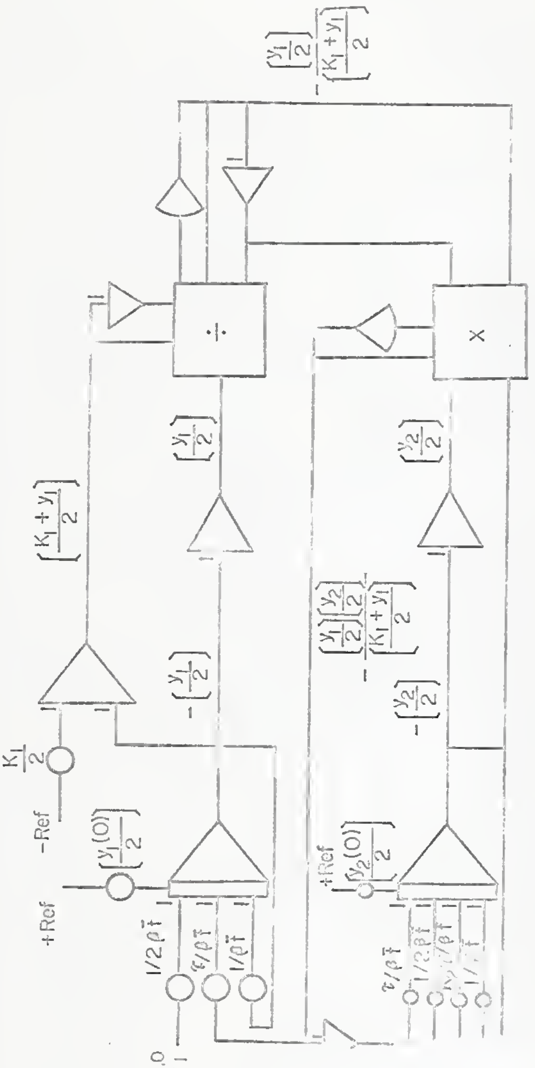

Fig. 7. Analog diagram for equations (44) and (45).

Table III

TR-48 Potentiometer Assignment Summary For Section 2 of Chapter 4 (see Figure 7)

Parameter description	Setting static check	Static check output voltage	Setting Run #1
$y_1(0)/2$	0.5	0.5	0.5
$y_2(0)/2$	0.5	0.5	0.0006*
$1/2\beta\bar{t}$	0.5	0.5	0.05
$\tau/\beta\bar{t}$	1.0	-0.455	1.0
$1/\beta\bar{t}$	1.0	-0.5	0.1
$\tau/\beta\bar{t}$	1.0	0.455	1.0
$1/2\beta\bar{t}$	0.0	0.0	0.0
$K_2\tau/\beta\bar{t}$	0.02	-0.01	0.02
$1/\beta\bar{t}$	1.0	-0.5	0.1
$K_1/2$	0.05	-0.05	0.05

*Initial condition of organism, $y_2(0)$, in the system is taken as 0.0012 since it is equivalent to a condition of innoculation of same bacteria in the plant.

Table IV

TR-48 Amplifier Assignment for Section 2 of Chapter 4 (see Figure 7)

FB	Output Variable	Static Check			
		Calculated		Measured	
		Deriv.	Output	Deriv.	Output
S	$-y_1/2$	-0.45	-0.5	0.4503	-0.5
S	$-y_2/2$	-0.05	-0.5	0.0546	-0.5
E	$(K_1+y_1)/2$	-	0.55	-	0.5498
I	$y_1/2$	-	0.5	-	0.5
I	$-(K_1+y_1)/2$	-	-0.55	-	-0.55
I	$-(\frac{y_1}{2})/(\frac{K_1+y_1}{2})$	-	0.91	-	0.9087
I	$y_2/2$	-	0.5	-	0.5
I	$(\frac{y_1}{2})(\frac{y_2}{2})/(\frac{K_1+y_1}{2})$	-	0.455	-	0.455
H	$-(\frac{y_1}{2})/(\frac{K_1+y_1}{2})$	-	-0.91	-	-0.9088
H	$-(\frac{y_1}{2})(\frac{y_2}{2})/(\frac{K_1+y_1}{2})$	-	-0.455	-	-0.4557

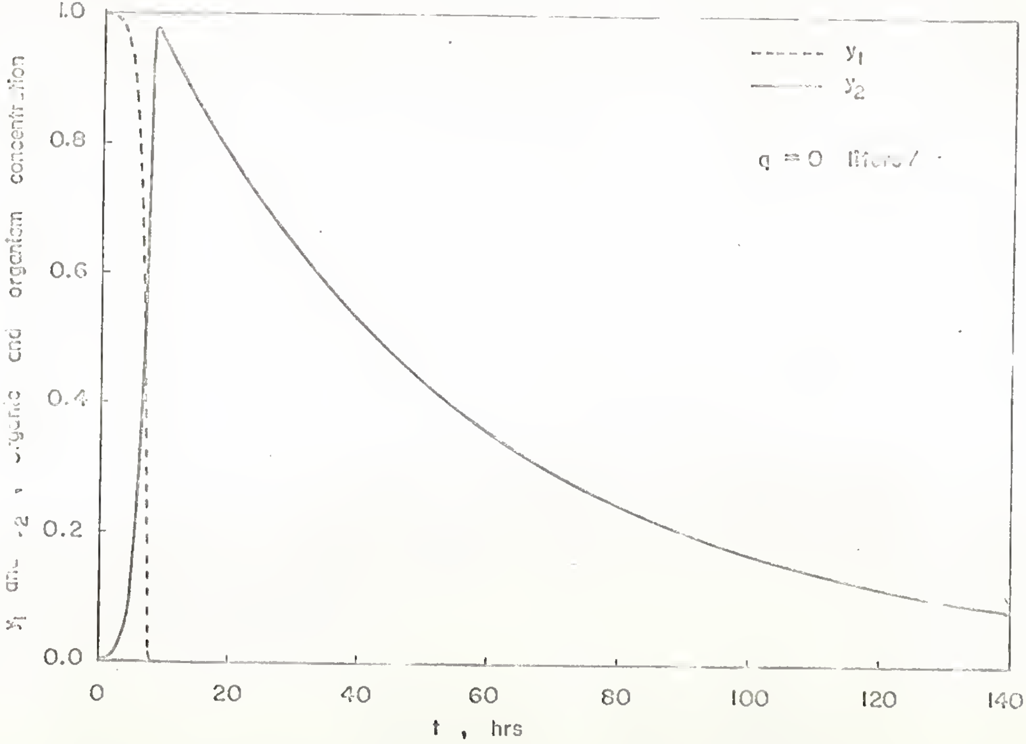

Fig. 8. Incomplete transient curves of organic and organism concentration for batch kinetics .

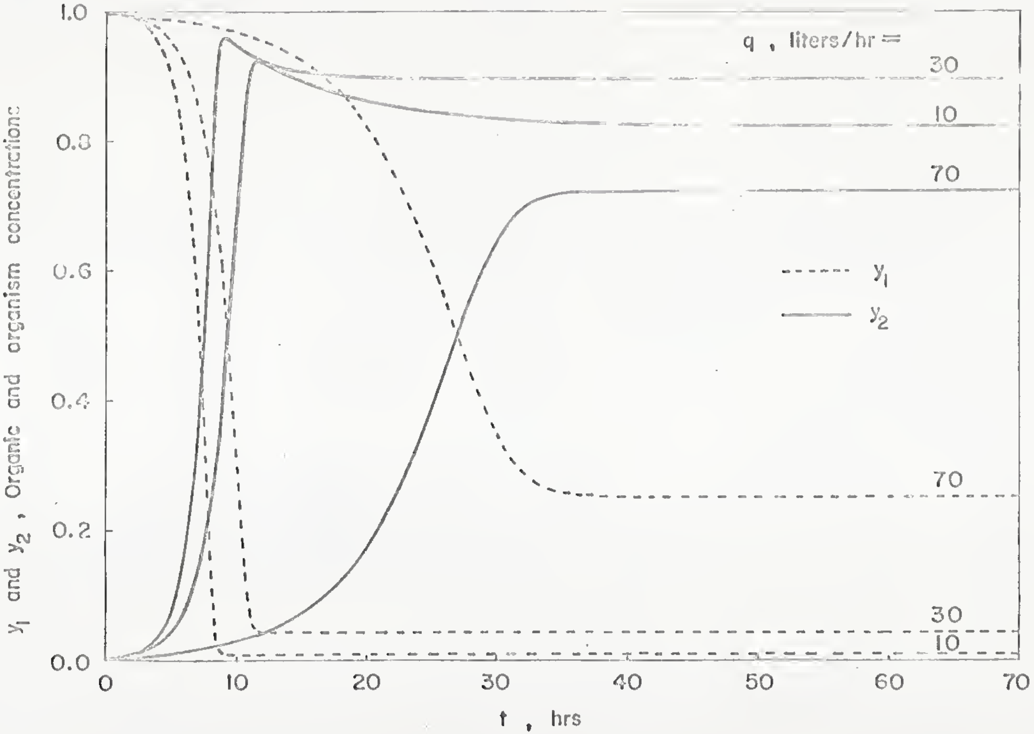

Fig. 9. Organic and organism concentration against time with flow rate as parameter.

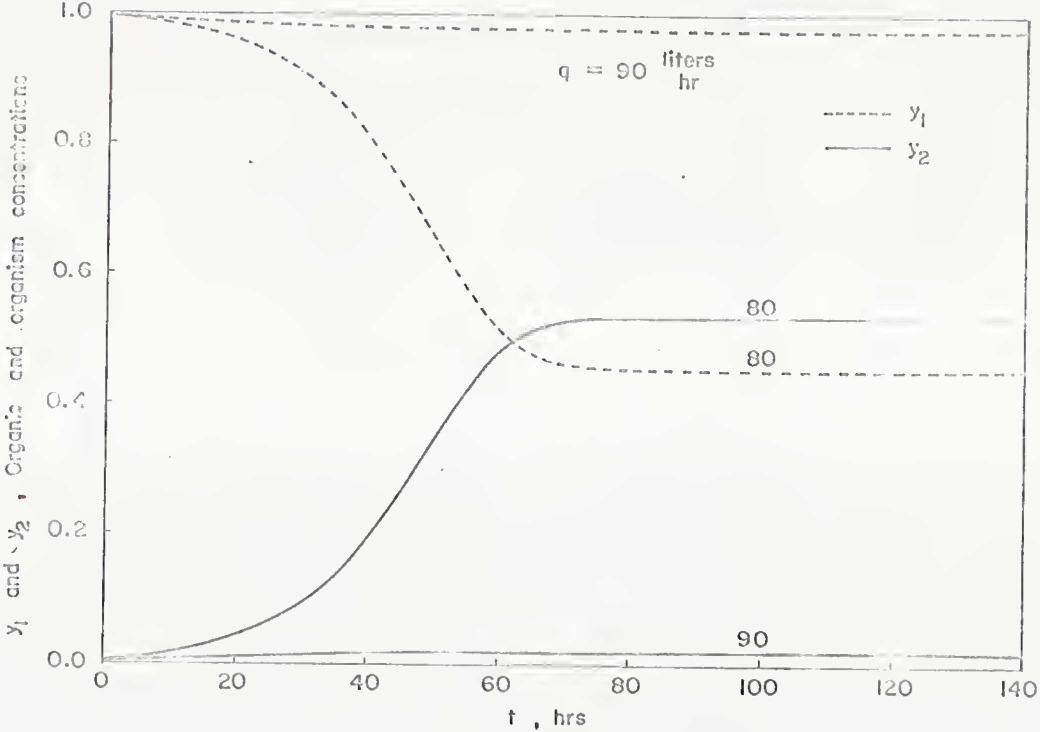

Fig. 10. Organic and organism concentration against time for flow rates near the washout condition.

the flow rate at which the washout condition ($y_1 \rightarrow 1$, $y_2 \rightarrow 0$) is approached. It should be noted that in section 4 of Chapter III, Part II, the minimum mean holding time corresponding to the washout condition has been calculated as 11.02 hrs. In other words, washout should occur near a flow rate of 90.8 liters/hr since the volume of the tank is assumed to be a 1000 liters. Hence, the analog computer result of $q = 90^+$ liters/hr for the near washout condition is in good agreement with the theoretical value obtained.

The time constants, that is, the time required by the system to reach 63.2% of the ultimate steady state value, are determined from Figures 9 and 10. In deriving these time constants, one has to assume that the system is a first order system. It can be seen from Figures 9 and 10 that the system responses are quite similar to those of the first order system. Hence, the time constants are derived for this system and are summarized in Table V.

Next, it is assumed that the plant is originally operated under a steady state condition with a flow rate of 80 liters/hr. A step change is introduced in the flow rate at t = 0 and as a result the organic and organism concentrations change with time as can be seen from Figures 11 and 12 respectively. This procedure is repeated for various step changes in the flow rate. It should be noted that theoretically the one stage isothermal completely mixed stirred tank reactor system does not completely attain the condition of washout from the normal operating condition because there are always some organisms remaining

Table V

Time Constants for the System with Constant x_1^0 and constant q.

Flow rate q, liters/hr	Time constant, time to reach 63.21% of the ultimate value, hrs.
10	9
30	10.6
70	30
80	55
90	40

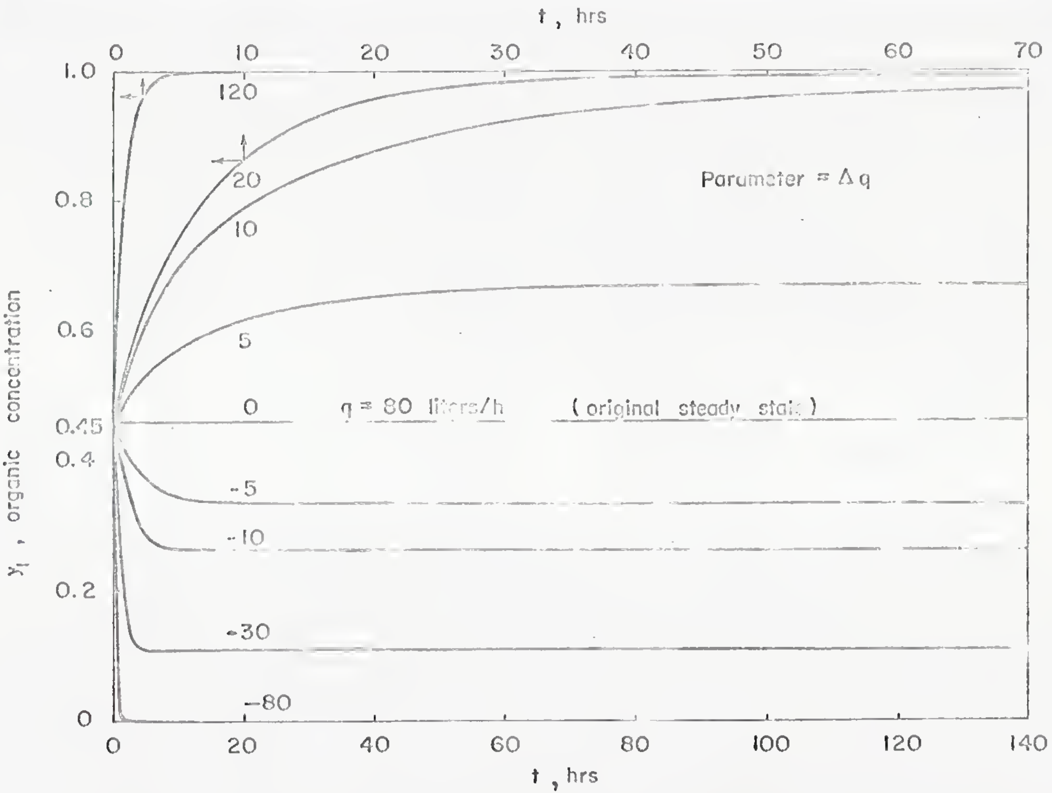

Fig. 11. Transient response of organic concentration for step change in flow rate .

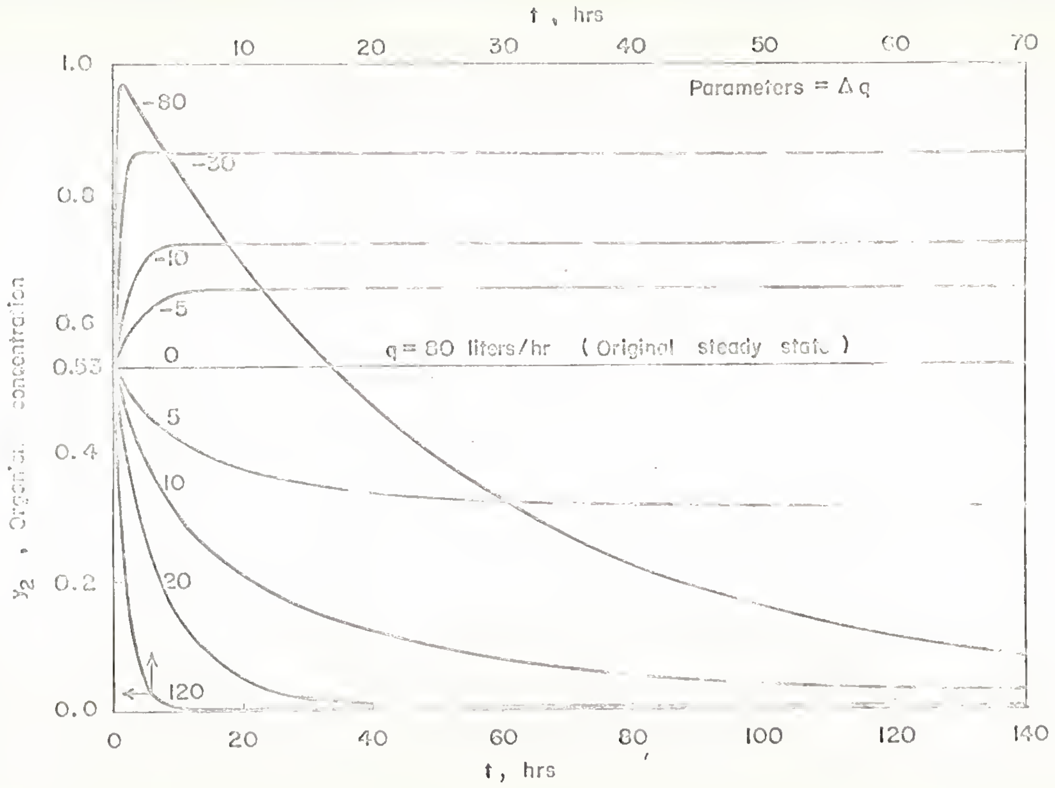

Fig. 12 . Transient response of the organism concentration for step change in flow rate .

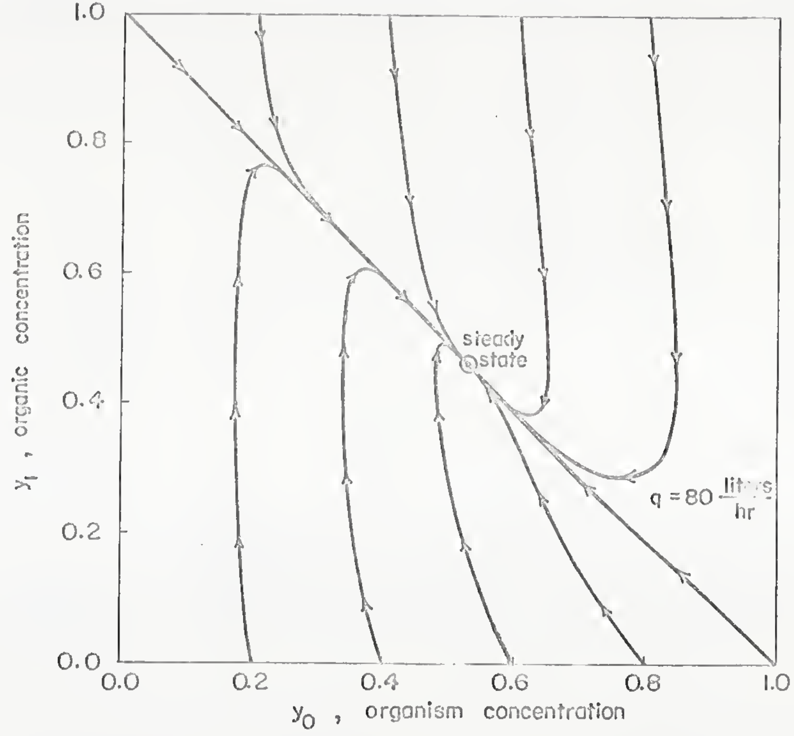

Fig. 13. Phase-plane plot for q = 80 liters/hr.

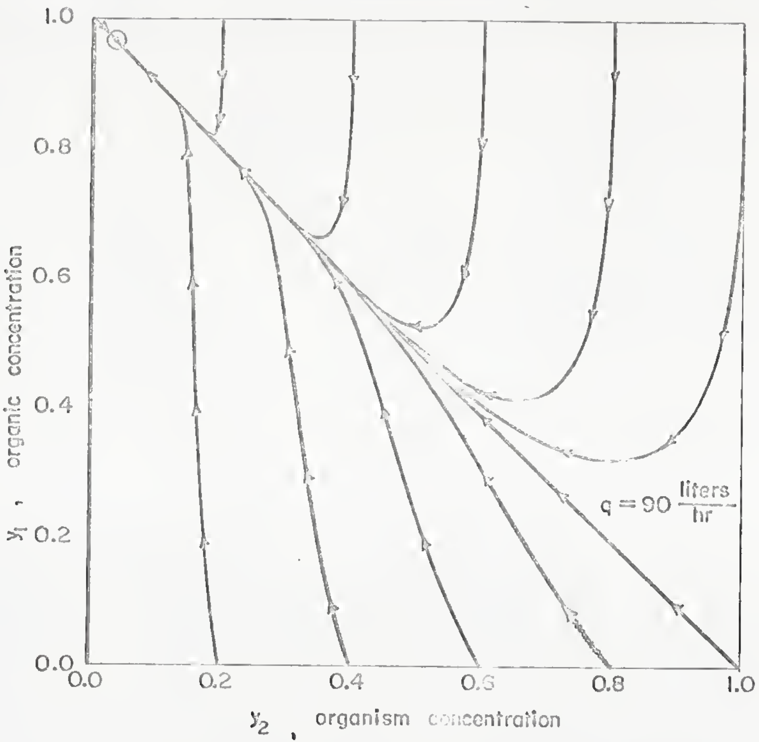

Fig. 14. Phase-plane plot for q = 90 liters/hr.

in the system. For example, even when the flow rate of 80 liters/hr is changed to the flow rate of 200 liters/hr which is far greater than the washout flow rate of 90.8 liters/hr, the system does not completely washout within a finite length of time. Furthermore, it is worth noting that the plug flow tubular reactor attains the condition of washout even when the flow rate is increased only slightly above the washout flow rate. The time required by the system to reach the washout condition is equal to the mean residence time. It is also worth noting that Figures 11 and 12 can also represent the condition of restart-up of the plant.

In Figures 13 and 14, the dimensionless organic concentration during the transient period is plotted against the corresponding dimensionless organism concentration by eliminating the independent time variable, t. These plots are known as phase-plane plots. Each point on these figures can be considered either as the condition of the system before start-up or the original steady state condition corresponding to a certain inflow condition. Therefore, each of these figures summarizes a part of the transient responses of Figures 9 through 12 and more. They can be considered to represent the transient responses during the start-up or restart-up period of the plant. That is, these figures show the relationship between y_1 and y_2 in the system while approaching the steady state condition from the initial start-up or restart-up condition. Figures 13 and 14 also show the responses of the system to a step change in the flow rate from the original one corresponding to a point on the figures to the new flow rate of 80 liters/hr. in Figure 13 and to the new flow rate of 90 liters/hr. in Figure 14 respectively. That is, these figures show that the relationships between y_1 and y_2 in the system during its new steady state valuc after introducing the step change in the flow rate.

3. RESPONSE OF THE SYSTEM TO A SINUSOIDAL DISTURBANCE IN THE INFLUENT ORGANIC CONCENTRATION

a. Performance Equations

In this section, responses of the system to sinusoidal variations of the influent organic concentration, x_1^0, are examined. The flow rate, q, of the influent is assumed to remain constant throughout the process.

The sinusoidal variation of the steady state influent organic concentration can be written as

$$x_1^0 = x_{1s}^0 + A \sin \omega_1 t \tag{46}$$

where

x_{1s}^0 = steady state influent organic concentration, mg/liter

A = amplitude of the sinusoidal variation, mg/liter

ω_1 = angular frequency of the sinusoidal disturbance, radians/hr.

$= 2\pi f_1$ where f_1 = cycles/hr.

Equation (46) can be rewritten as

$$\frac{x_1^0}{x_{1s}^0} = 1 + A_1 \sin \omega_1 t \tag{47}$$

where A_1 is the dimensionless amplitude of the sinusoidal variation and is defined as

$$A_1 = \frac{A}{x_{1s}^0}$$

The dimensionless influent organic concentration is defined as

$$y_1^0 = \frac{x_1^0}{x_{1s}^0} \tag{48}$$

and hence from Equation (47), one has

$$y_1^0 = 1 + A_1 \sin \omega_1 t \tag{49}$$

In this problem, dimensionless variables and parameters must be based on the steady state influent organic concentration as originally defined, that is,

$$y_1 = \frac{x_1}{x_{1s}^0}, \quad y_2 = \frac{x_2}{Yx_{1s}^0}, \quad K_1 = \frac{K}{x_{1s}^0}$$

Then the following performance equations of the system, which are similar to Equations (42) and (43) are obtained from Equations (9) and (11).

$$\frac{dy_1}{dt} = (1 + A_1 \sin \omega_1 t - y_1)\,\frac{1}{\bar{t}} - \frac{\tau}{\bar{t}}\,\left(\frac{y_1\,y_2}{K_1+y_1}\right) \tag{50}$$

and

$$\frac{dy_2}{dt} = (y_2^0 - y_2)\frac{1}{\bar{t}} + \frac{\tau}{\bar{t}}\left(\frac{y_1\ y_2}{K_1 + y_1} - K_2\ y_2\right) \qquad (51)$$

It is worth noting that because the dimensionless variables are defined on the basis of steady state influent organic concentration, x_{1s}^0, the value of these dimensionless variables may go higher than one.

b. Scaling and Static Test for Analog Computer

The magnitude scalings for the system variables are the same as those previously summarized in Table II. The only exception is for

$$y_1^0 = 1 + A_1 \sin \omega_1 t$$

Note that y_1^0 is also the output of an amplifier and, therefore, must be scaled. Since the range of A_1 is zero to one (that is, 0% to 100% variation), one can expect that the maximum value of $(1 + A_1 \sin \omega_1 t)$ is two. Therefore, the corresponding computer variable should be

$$\left[\frac{1 + A_1 \sin \omega_1 t}{2}\right]$$

Therefore, the scaled performance equations for this problem are

$$\frac{d\left[\frac{y_1}{2}\right]}{dt} = \left(\frac{1}{\beta\bar{t}}\right)\left[\frac{1 + A_1 \sin \omega_1 t}{2}\right] - \left(\frac{1}{\beta\bar{t}}\right)\left[\frac{y_1}{2}\right] - \left[\frac{\tau}{\beta\bar{t}}\right]\frac{\left[\frac{y_1}{2}\right]\left[\frac{y_2}{2}\right]}{\left[\frac{K_1 + y_1}{2}\right]} \qquad (52)$$

and

$$\frac{d[\frac{y_2}{2}]}{dt} = (\frac{1}{2\beta\bar{t}})\, y_2^0 - (\frac{1}{\beta\bar{t}})[\frac{y_2}{2}] + (\frac{\tau}{\beta\bar{t}}) \frac{[\frac{y_1}{2}][\frac{y_2}{2}]}{[\frac{K_1 + y_1}{2}]} - (\frac{k_2\tau}{\beta\bar{t}})[\frac{y_2}{2}] \tag{53}$$

All the values of parameters and constants are the same as those employed in the preceding sections.

Figure 15 shows the scaled analog diagram for the analog computation. The pot settings for the static test and for the actual run are summarized in Table VI. The output voltages for each pot and each amplifier for the static test are also shown in Tables VI and VII respectively.

c. Results and Discussion

The response of the system to sinusoidal variations of the influent organic concentration is shown in Figures 16 through 23. The sinusoidal variation of the inflow organic concentration is also shown for each case in order to indicate the amplitude and frequency of the variation. It is assumed that the system is operating under steady state condition at a flow rate of 80 liters/hr before the initiation of the disturbance. Since the size of the reactor is assumed to be 1000 liters, this flow rate corresponds to a mean holding time of 12.5 hours. The steady state value of the influent organic concentration x_{1s}^0, is 200 mg/liter as mentioned previously.

In the first four cases, shown in Figures 16 through 19, the

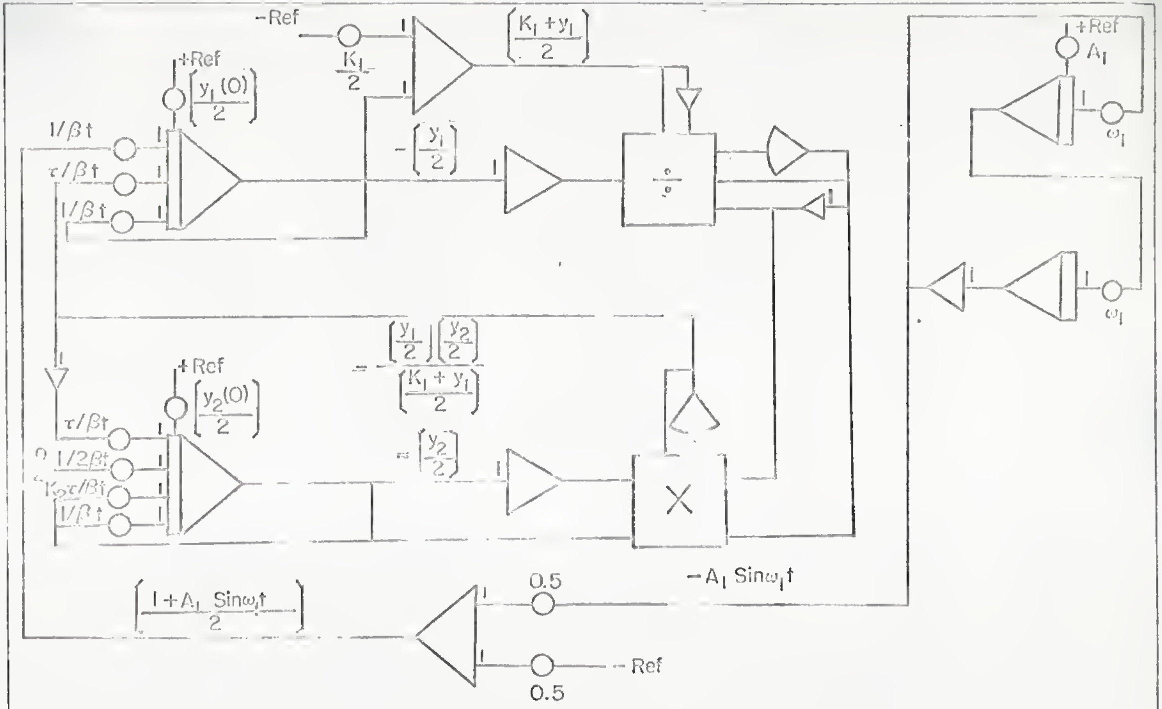

Fig. 15. Analog diagram for equations (52) and (53).

Table VI

TR-48 Potentiometer Assignment Summary for section 3 of chapter 4 (See Figure 15)

Parameter Description	Setting Static Check	Static Check Output Voltage	Setting Run #1
$y_1(0)/2$	0.5	0.5	0.2264*
$y_2(0)/2$	0.5	0.5	0.2668*
I. C. for Static Check	1.0	-1.0	0.0
$1/\beta\bar{t}$	1.0	1.0	0.8
$\tau/\beta\bar{t}$	1.0	-0.544	1.0
$1/\beta\bar{t}$	1.0	-0.5	0.8
$\tau/\beta\bar{t}$	1.0	0.455	1.0
$k_2\tau/\beta\bar{t}$	0.02	-0.01	0.02
$1/\beta\bar{t}$	1.0	-0.5	0.8
$k_1/2$	0.05	-0.05	0.05
A_1	1.0	-1.0	0.2
w_1	1.0	-1.0	1.0
w_1	1.0	-1.0	1.0
Const.	0.5	-0.5	0.5
Const.	0.5	-0.5	0.5

*The system is operating under the steady state condition at flow rate of 80 liters/hr and these initial values represent the steady state organic and organism concentrations respectively.

Table VII

TR-48 Amplifier Assignment Summary for section 3 of chapter 4

		Static Check			
FB	Output	Calculated		Measured	
	Variable	Deriv.	Output	Deriv.	Output
S	$-y_1/2$	-0.045	-0.5	0.0476	-0.5
S	$-y_2/2$	-0.055	-0.5	0.055	-0.5
S	$A_1 \sin \omega_1 t$	-1.0	1.0	1.0	1.0
S	$-A \sin \omega_1 t$	-1.0	-1.0	1.0	-1.0
E	$(K_1 + y_1)/2$	-	0.55	-	0.55
E	$(1+A_1 \sin \omega_1 t)/2$	-	1.0	-	1.0
I	$y_1/2$	-	0.5	-	0.5
I	$-(K_1+y_1)/2$	-	-0.55	-	-0.55
I	$(\frac{y_1}{2})/(\frac{K_1 + y_1}{2})$	-	0.91	-	-0.9088
I	$-A_1 \sin w_1 t$	-	-1.0	-	-1.0
I	$y_2/2$	-	0.5	-	0.5
I	$(\frac{y_1}{2})(\frac{y_2}{2})/(\frac{K_1+y_1}{2})$	-	0.455	-	0.454
H	$-(\frac{y_1}{2})/(\frac{K_1 + y_1}{2})$	-	0.91	-	-0.908
H	$-(\frac{y_1}{2})(\frac{y_2}{2})/(\frac{K_1+y_1}{2})$	-	-0.455	-	-0.455

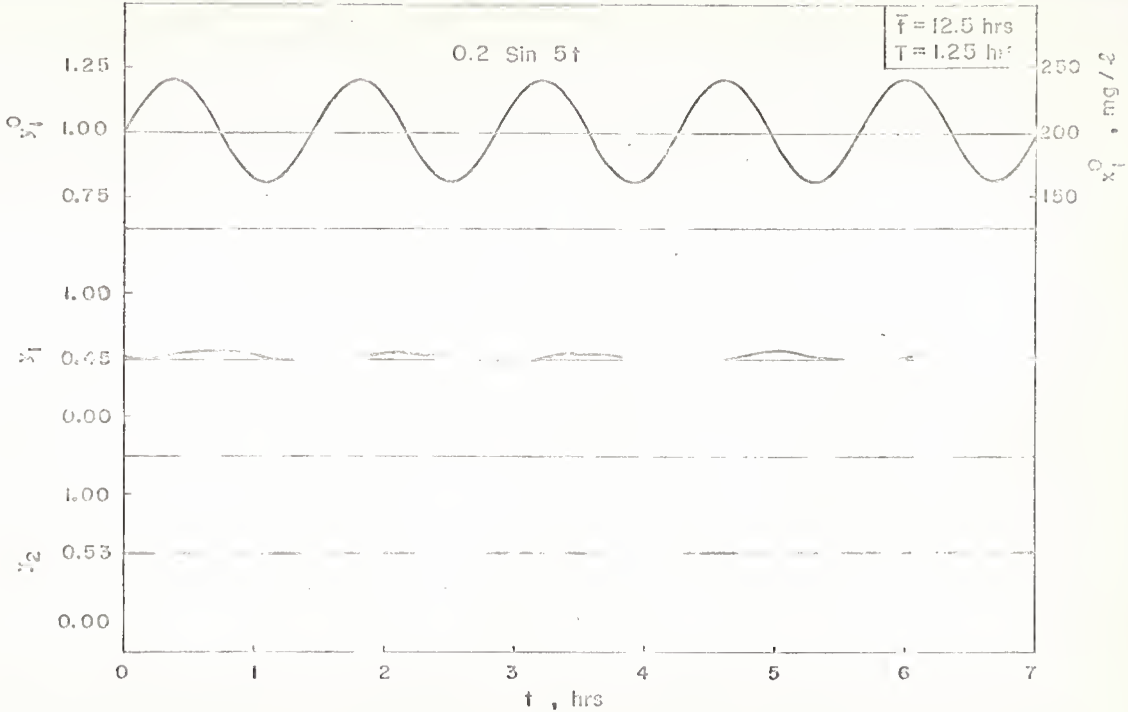

Fig. 16. Response of the system to a sinusoidal variation in the influent organic concentration for $A_1 = 0.2$ and $\omega_1 = 5.0$.

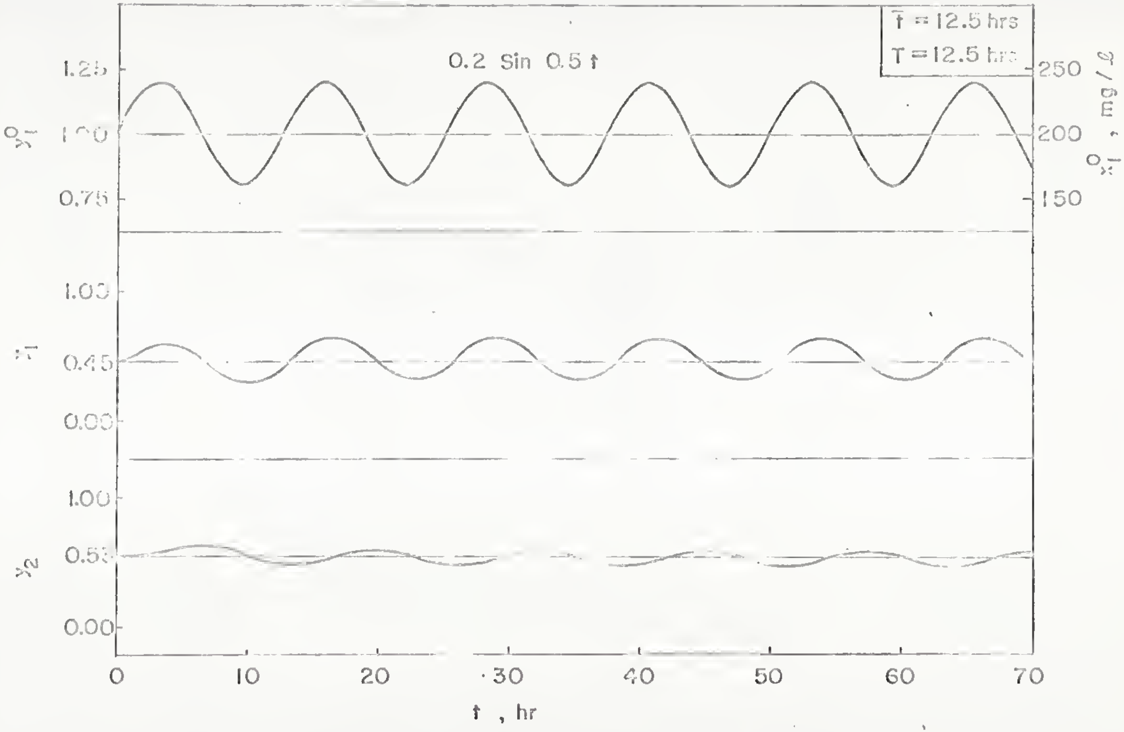

Fig. 17. Response of the system to a sinusoidal variation in the influent organic concentration for $A_1 = 0.2$ and $\omega_1 = 0.5$.

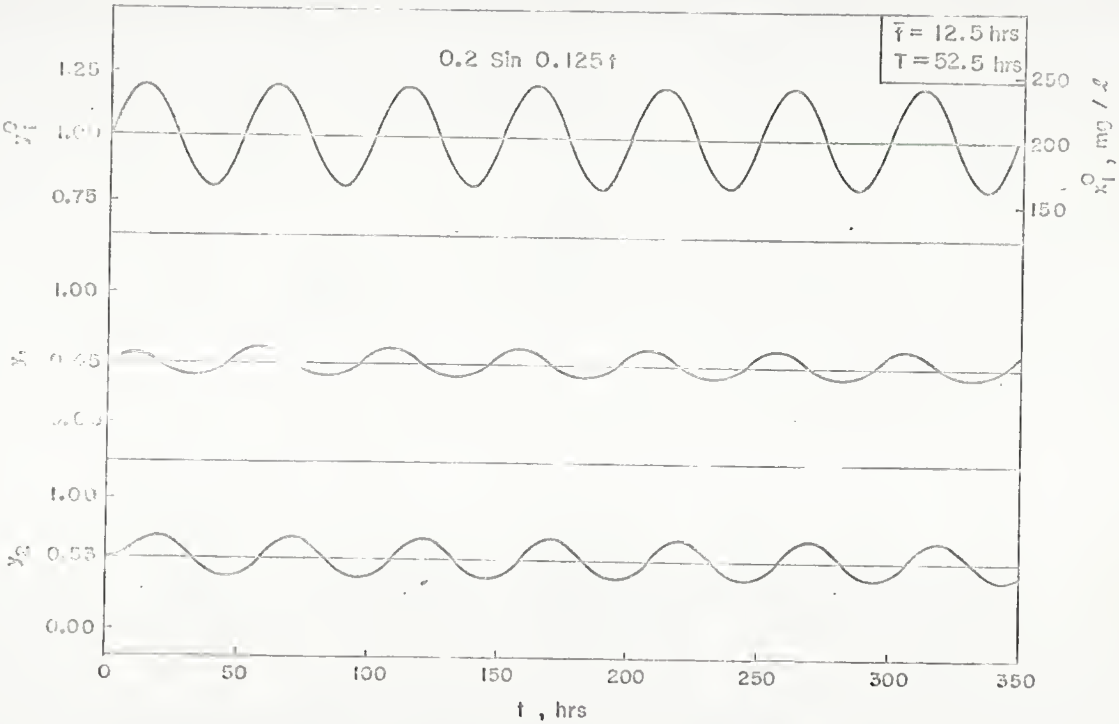

Fig. 18. Response of the system to a sinusoidal variation in the influent organic concentration for $A_1 = 0.2$ and $\omega_1 = 0.125$.

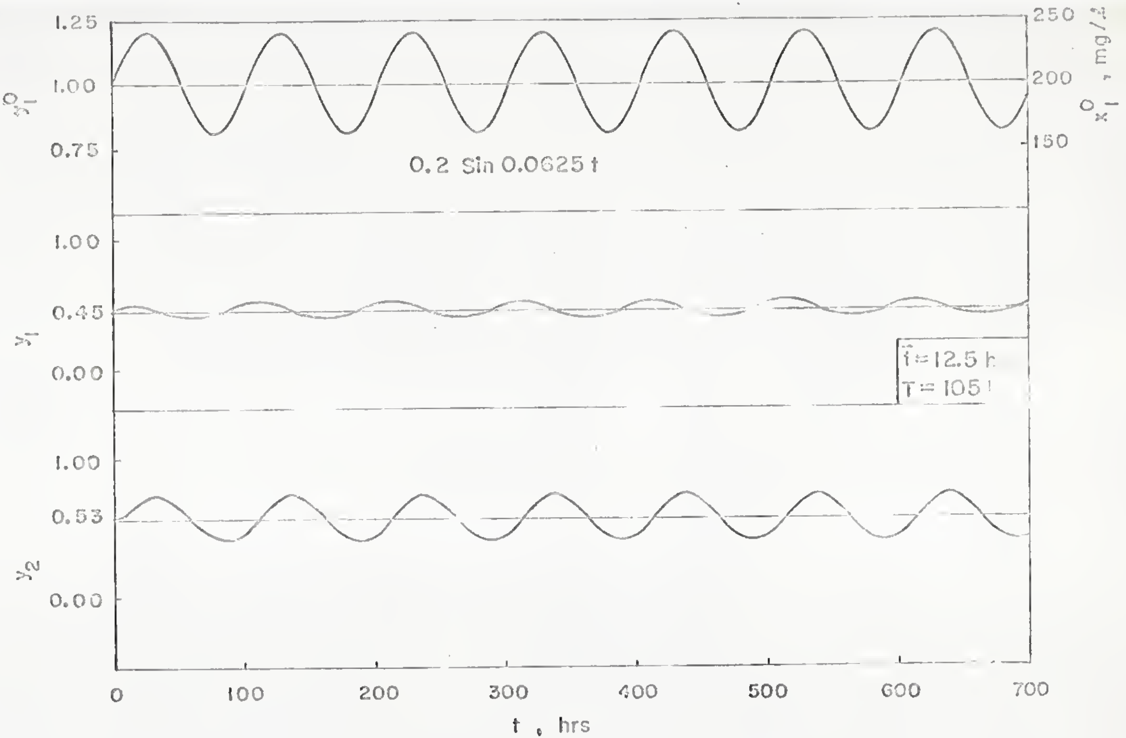

Fig. 19. Response of the system to a sinusoidal variation in the influent organic concentration for $A_1 = 0.2$ and $\omega_1 = 0.0625$.

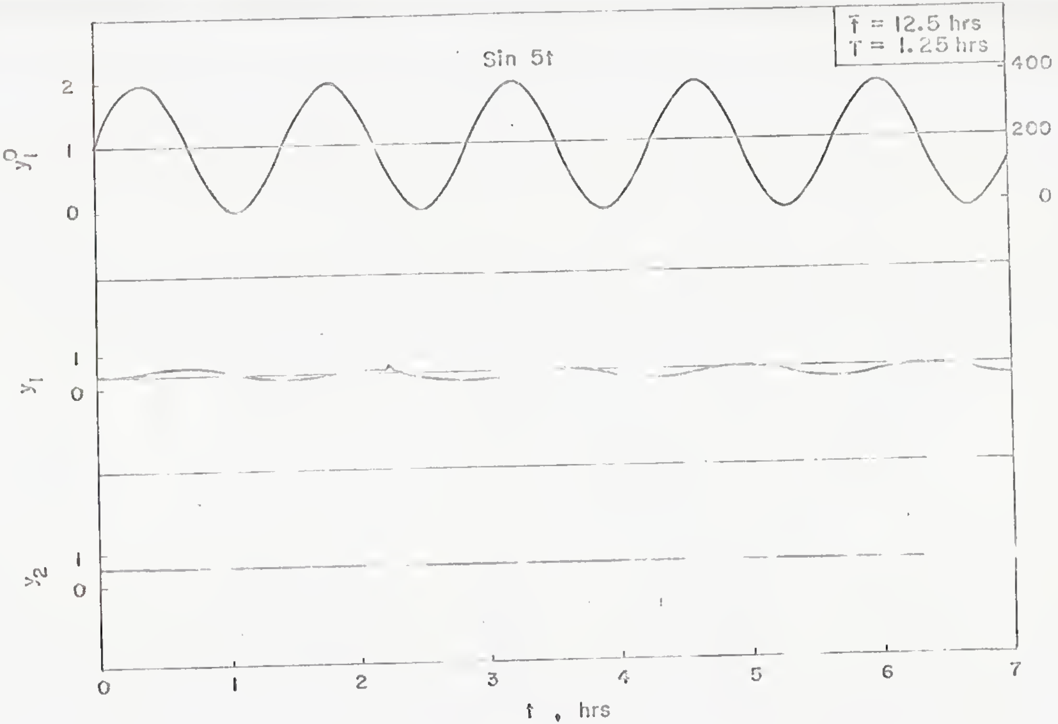

Fig. 20. Response of the system to a sinusoidal variation in the influent organic concentration for $A_1 = 1$ and $\omega_1 = 5.0$.

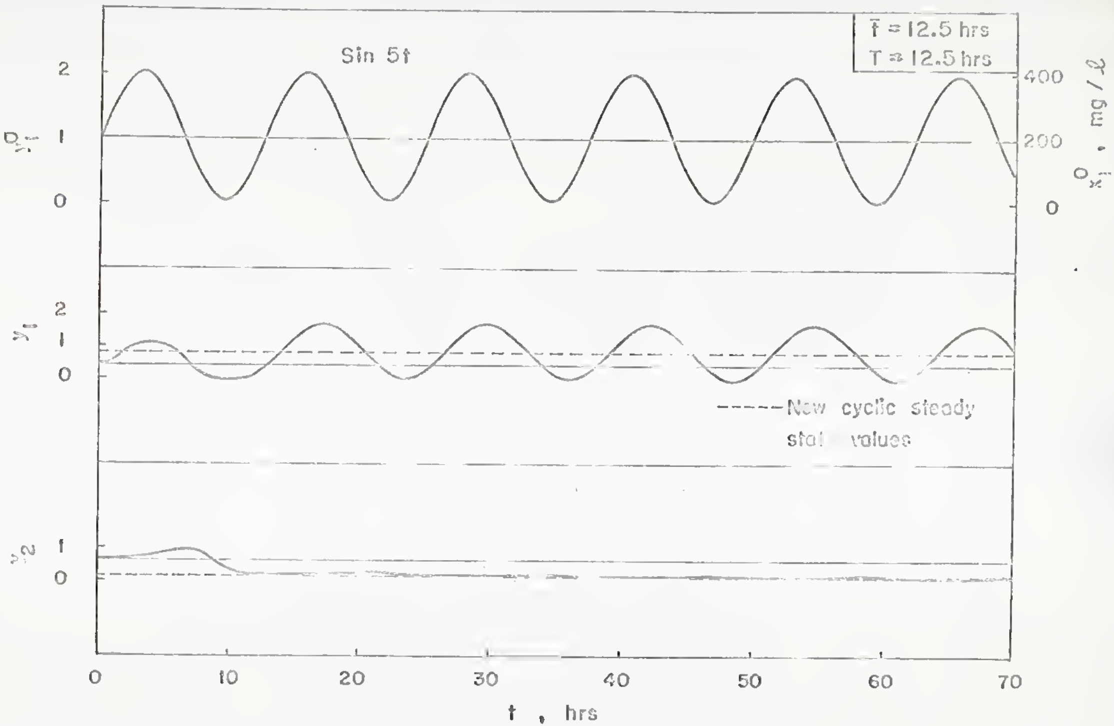

Fig. 21. Response of the system to a sinusoidal variation in the influent organic concentration for $A_1 = 1$ and $\omega_1 = 0.5$.

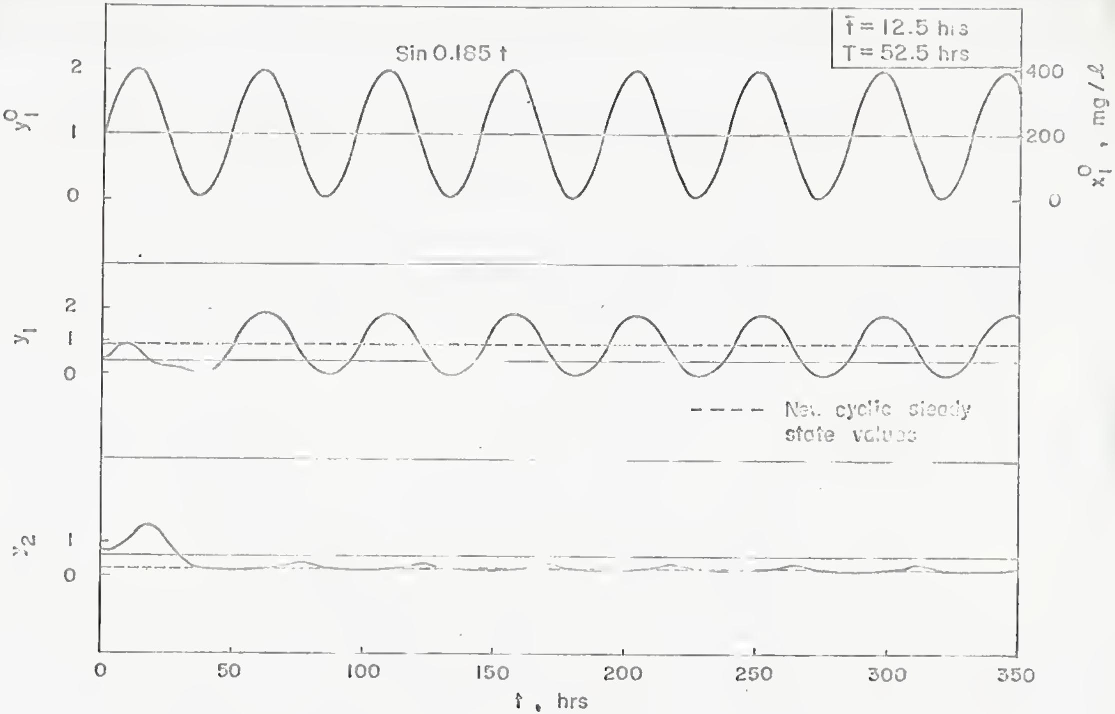

Fig. 22. Response of the system to a sinusoidal variation in the influent organic concentration for $A_1 = 1$ and $\omega_1 = 0.125$.

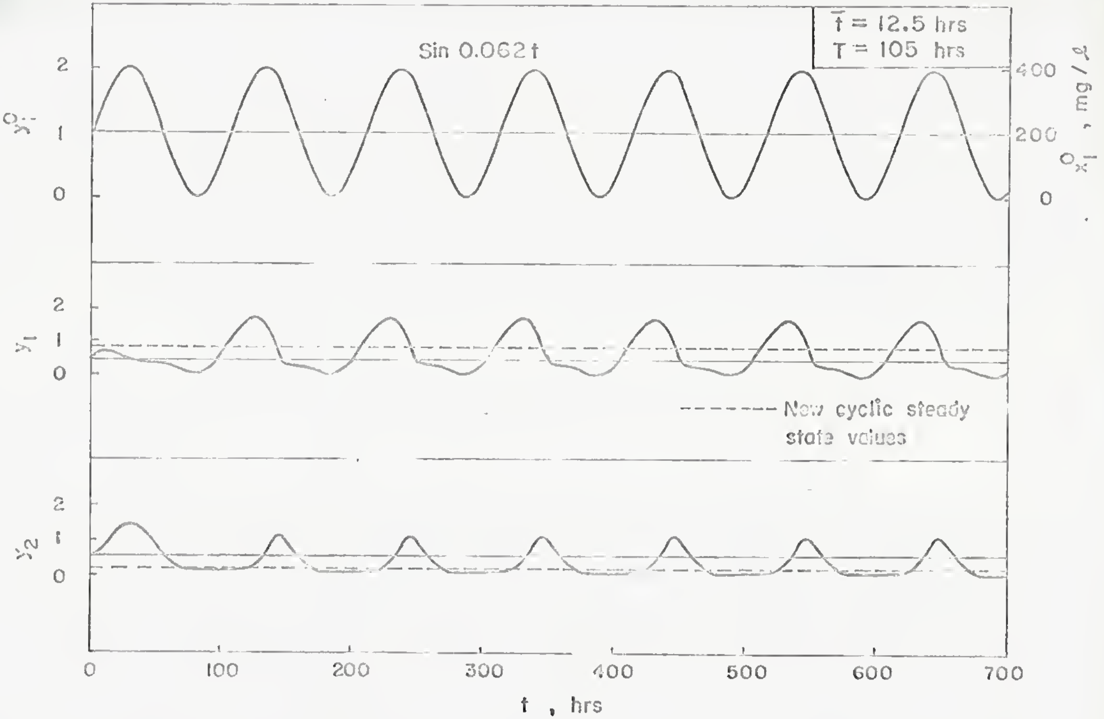

Fig. 23. Response of the system to a sinusoidal variation in the influent organic concentration for $A_1 = 1$ and $\omega_1 = 0.0625$.

amplitude of the sinusoidal fluctuation of x_1^0 remained constant at a value of twenty percent of the initial steady-state value. This corresponds to a dimensionless amplitude, A_1, of 0.2 or to a range of sinusoidal fluctuation of influent organic concentration between 160 to 240 mg/liter. With this amplitude, the angular frequency, ω_1, of fluctuation was varied from 5.0 radian/hr to 0.0625 radian/hr., corresponding to a period of fluctuation ranging from one tenth of the mean holding time to approximately ten times the mean holding time.

In the second four cases shown in Figures 20 through 23, the amplitude of the fluctuation of the influent organic concentration is 100% of the initial steady state influent organic concentration. This corresponds to a range of the steady state influent organic concentration between 0 and 400 mg/liter.

Figure 16 shows that at a high frequency of fluctuation (period of oscillation of the order of a tenth of the mean holding time of the system), the values of the organic concentration, y_1, and the organism concentration, y_2, are not appreciably affected and essentially remain at the original steady state values.

From Figures 17 through 19, however, one can generally see that as the frequency is reduced (period of oscillation becoming larger), the effect of the magnitude of the variation of x_1^0 on system variables is increased. At a period of oscillation corresponding to the mean holding time (see Figure 17) the effect of the variation on the magnitude of the organic concentration is more apparent than that on the organism concentration. However, the mean values of the system variables essentially remain at the original steady state values. As the frequency becomes much smaller (or as the period of oscillation becomes much larger than the mean holding time), as shown in Figures 18 and 19, the effect of the disturbance on the organism concentration becomes more appreciable than that on the organic concentration. However, the mean values of the system variables still remain essentially at the original steady state values.

Figure 20 shows that even though the fluctuation in x_1^0 is increased to 100%, the values of the organic and organism concentrations are not appreciably affected at a very high frequency of oscillation. However, the organic concentration is reduced slightly to a new cyclic steady state value. As the frequency is reduced, the non-linearity of the system becomes apparent as can be seen from Figures 21 through 23. It is also observed from these figures that the organic concentration reaches a new cyclic steady state value which is higher than the original steady state value, and the organism concentration reaches a new cyclic steady state value which is lower than the original steady state value. It can be generally concluded that a very high fluctuation in x_1^0 would reduce the capacity of the system especially if the frequency of the fluctuation is low.

It is also worth noting again that the dimensionless concentrations can exceed unity since they are all defined on the basis of steady state influent organic concentration.

4. RESPONSE OF THE SYSTEM TO A SINUSOIDAL DISTURBANCE IN THE FLOW RATE

a. Performance Equations

In this section responses of the system to sinusoidal variations of the influent flow rate, q, are observed. It is assumed that the influent organic concentration remains constant throughout the process at the steady state value of x_{1s}^0.

The sinusoidal variation of the influent flow rate can be written as

$$q = q_s + B \sin \omega_2 t \tag{54}$$

where

q_s = steady state flow rate, liters/hr.

B = amplitude of the sinusoidal disturbance, liters/hr

ω_2 = angular frequency of the sinusoidal disturbance, radians/hr.

$= 2\pi f_2$, where f_2 = cycles/hr.

Equation (54) can be rewritten as

$$\frac{q}{q_s} = 1 + A_2 \sin \omega_2 t \tag{55}$$

where A_2 is the dimensionless amplitude of the sinusoidal variation and is defined as

$$A_2 = \frac{B}{q_s}$$

Equations (42) and (43) which are the performance equations of the system under consideration can be rewritten as

$$\frac{dy_1}{dt} = (y_1^0 - y_1)\frac{q_s/q_s}{V/q} - (\frac{\tau}{\bar{t}})(\frac{y_1\,y_2}{K_1+y_1}) \tag{56}$$

and

$$\frac{dy_1}{dt} = (y_2^0 - y_2)\frac{q_s/q_s}{V/q} + (\frac{\tau}{\bar{t}})(\frac{y_1\,y_2}{K_1+y_1} - K_2\,y_2) \tag{57}$$

respectively. It should be noted that the ratio of τ to $\bar{t}$, is a constant and does not depend on the flow rate since

$$\frac{\tau}{\bar{t}} = \frac{k\bar{t}}{t} = k$$

Now, if the steady state mean holding time is defined as

$$\bar{t}_s = \frac{V}{q_s}, \tag{58}$$

Equations (56) and (57) can be rewritten with the help of Equation (55) as

$$\frac{dy_1}{dt} = (1 + A_2 \sin \omega_2 t)\frac{y_1^0}{\bar{t}_s} - (1 + A_1 \sin \omega_2 t)\frac{y_1}{\bar{t}_s} - (\frac{\tau}{\bar{t}})(\frac{y_1\,y_2}{K_1+y_1}) \tag{59}$$

and

$$\frac{dy_2}{dt} = (1 + A_2 \sin \omega_2 t)\frac{y_2^0}{\bar{t}_s} - (1 + A_2 \sin \omega_2 t)\frac{y_2}{\bar{t}_s} + (\frac{\tau}{\bar{t}})(\frac{y_1\,y_2}{K_1+y_1}) - (\frac{\tau}{\bar{t}})(K_2 y_2) \tag{60}$$

respectively.

b. Scaling and Static Test for Analog Computer

The magnitude scaling for the system variables remains the same as those in the preceding two sections. Hence, the scaled performance equations are obtained as

$$\frac{d\left[\frac{y_1}{2}\right]}{dt} = \left(\frac{1}{\beta\bar{t}_s}\right)\left[\frac{1 + A_2 \sin \omega_2 t}{2}\right] y_1^0 - 2\left(\frac{1}{\beta\bar{t}_s}\right)\left[\frac{1 + A_2 \sin \omega_2 t}{2}\right]\left[\frac{y_1}{2}\right]$$

$$- \left(\frac{\tau}{\beta\bar{t}}\right) \frac{\left[\frac{y_1}{2}\right]\left[\frac{y_2}{2}\right]}{\left[\frac{K_1 + y_1}{2}\right]} \qquad (61)$$

and

$$\frac{d\left[\frac{y_2}{2}\right]}{dt} = \left(\frac{1}{\beta\bar{t}_s}\right)\left[\frac{1 + A_2 \sin \omega_2 t}{2}\right] y_2^0 - 2\left(\frac{1}{\beta\bar{t}_s}\right)\left[\frac{1 + A_2 \sin \omega_2 t}{2}\right]\left[\frac{y_2}{2}\right]$$

$$+ \left(\frac{\tau}{\beta\bar{t}}\right) \frac{\left[\frac{y_1}{2}\right]\left[\frac{y_2}{2}\right]}{\left[\frac{K_1 + y_1}{2}\right]} - \left(\frac{K_2\tau}{\beta\bar{t}}\right)\left[\frac{y_2}{2}\right] \qquad (62)$$

respectively. All the values of the parameters and constants are kept the same as in the preceding two sections.

The scaled analog diagram for the analog computation is shown in Figure 24.

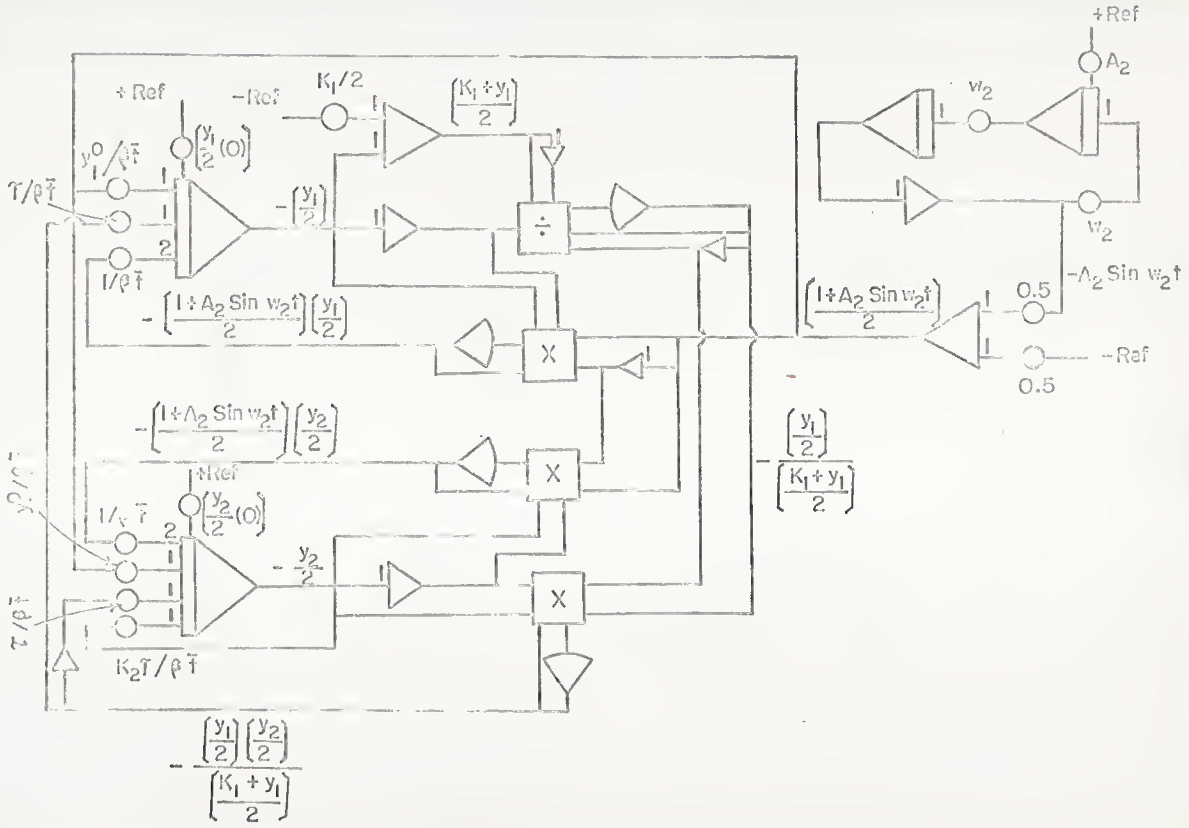

Fig. 24. Analog diagram for equations (61) and (62).

c. Results and Discussion

The response of the system to the sinusoidal variations of the influent flow rate, q, is shown in Figures 25 through 32. The sinusoidal variation of q is also shown for each case in order to indicate the amplitude and frequency of variation. It is assumed that in each case the system is operated under steady state conditions with a washout flow rate of 90 liters/hr. prior to initiating the disturbance. This particular flow rate is selected so that the effect of influent flow rate disturbance can be examined near the washout condition, which is a critical condition of the process. Since the size of the reactor is assumed to be 1000 liters, the influent flow rate of 90 liters/hr. corresponds to the mean holding time of 11.1 hrs.

In the first four cases, shown in Figures 25 through 28, the amplitude of disturbance remains constant at a value of 20% of the initial steady state value; that is, q oscillates approximately between 68 and 113 liters/hr. The period of oscillation is increased from about one tenth of the mean holding time to about ten times of the mean holding time.

Figure 25 shows that at a very high frequency of oscillation (or for a period of oscillation of one tenth of the mean holding time), the performance of the system is hardly affected and remains practically at its initial steady state condition. When the period of oscillation is equal to the mean holding time (see Figure 26), the performance of the system is very slightly affected. However, one can see from

Figures 27 and 28 that as the frequency of disturbance is lowered, the non-linearity of the system reveals itself very appreciably and the performance of the system is definitely affected. It should also be noted that the average value between the maximum and minimum of organic concentrations in both cases is approximately 0.75 and similarly that for the organism concentration is 0.25. The time averages of both quantities are nearer to the original steady state values than the values reported above.

In the second four cases shown in Figures 29 through 32, the amplitude of disturbance of the influent flow rate is 100%. This corresponds to the oscillation of q between 0 and 180 liters/hr.

Figure 29 shows that even though the disturbance of q is increased to 100%, the performance of the system is hardly affected at a very high rate of oscillation. As the frequency is reduced, the non-linearity of the system becomes apparent as can be seen from Figures 30 through 32. Deviations of the mean average values of the organic and organism concentrations from the original steady state increase with the increase of the amplitude of fluctuation (compare Figures 26, 27, and 28 with Figures 30, 31, and 32 respectively).

It can generally be concluded that the sinusoidal variation of the influent flow rate improves appreciably the performance of the system near the washout condition especially when the period of fluctuation is large. (This improvement may also be attained under other conditions). This may be considered as an advantageous application of

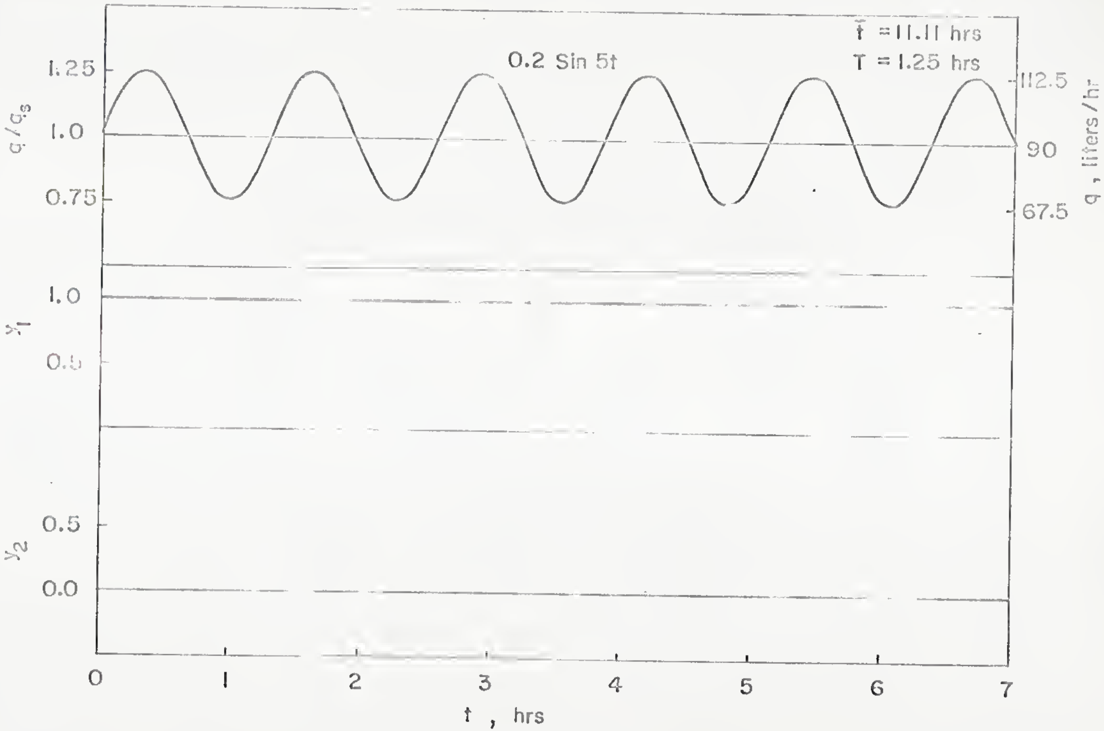

Fig. 25. Response of the system to a sinusoidal variation in the flow rate for $A_2 = 0.25$ and $w_2 = 5$.

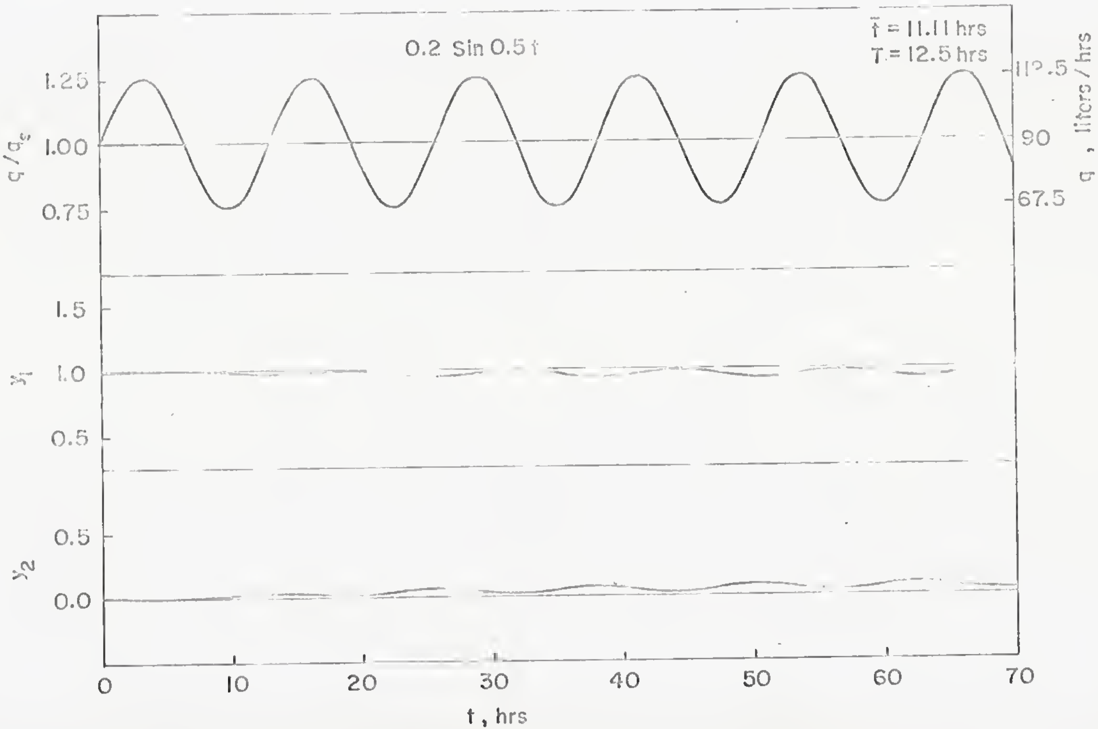

Fig. 26. Response of the system to a sinusoidal variation in the flow rate for $A_2 = 0.25$ and $w_2 = 0.5$.

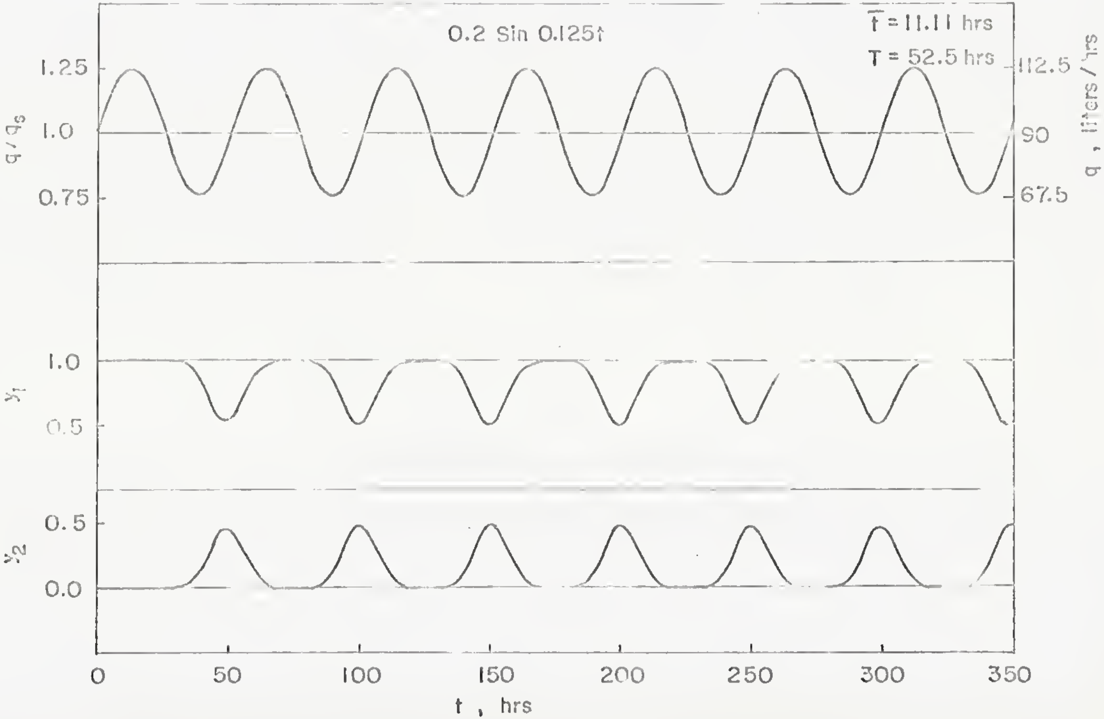

Fig. 27. Response of the system to a sinusoidal variation in the flow rate for $A_2 = 0.25$ and $w_2 = 0.125$.

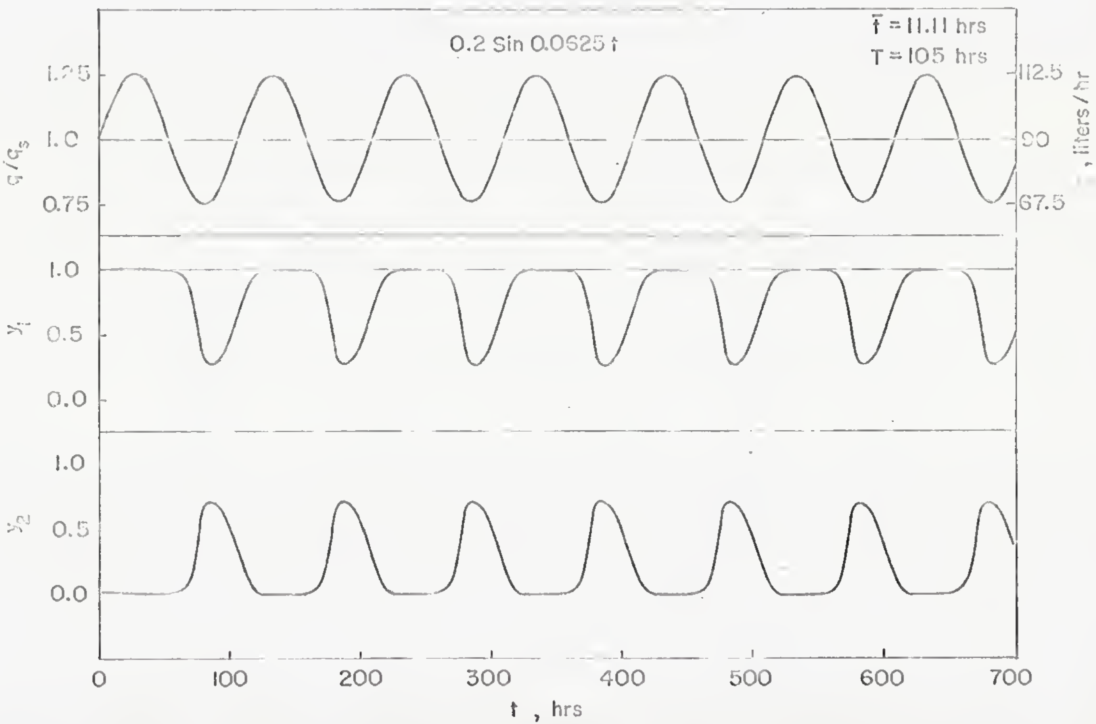

Fig. 28. Response of the system to a sinusoidal variation in the flow rate for $A_2 = 0.25$ and $w_2 = 0.0625$.

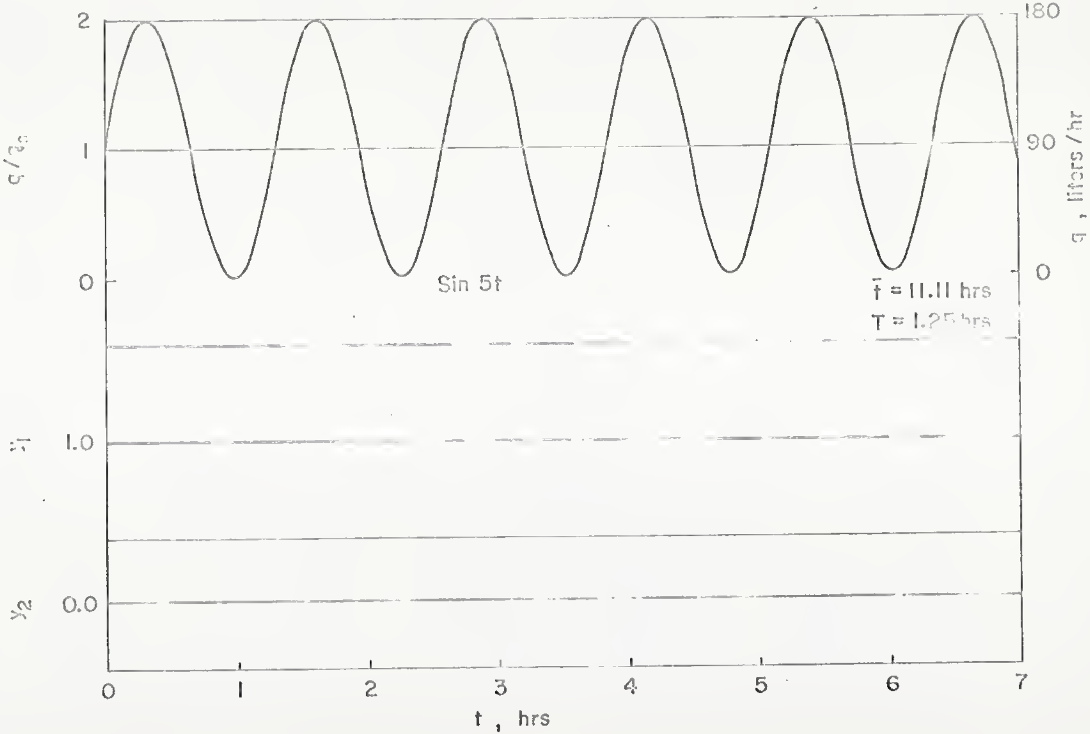

Fig. 29. Response of the system to a sinusoidal variation in the flow rate for $A_2 = 1$ and $w_2 = 5$.

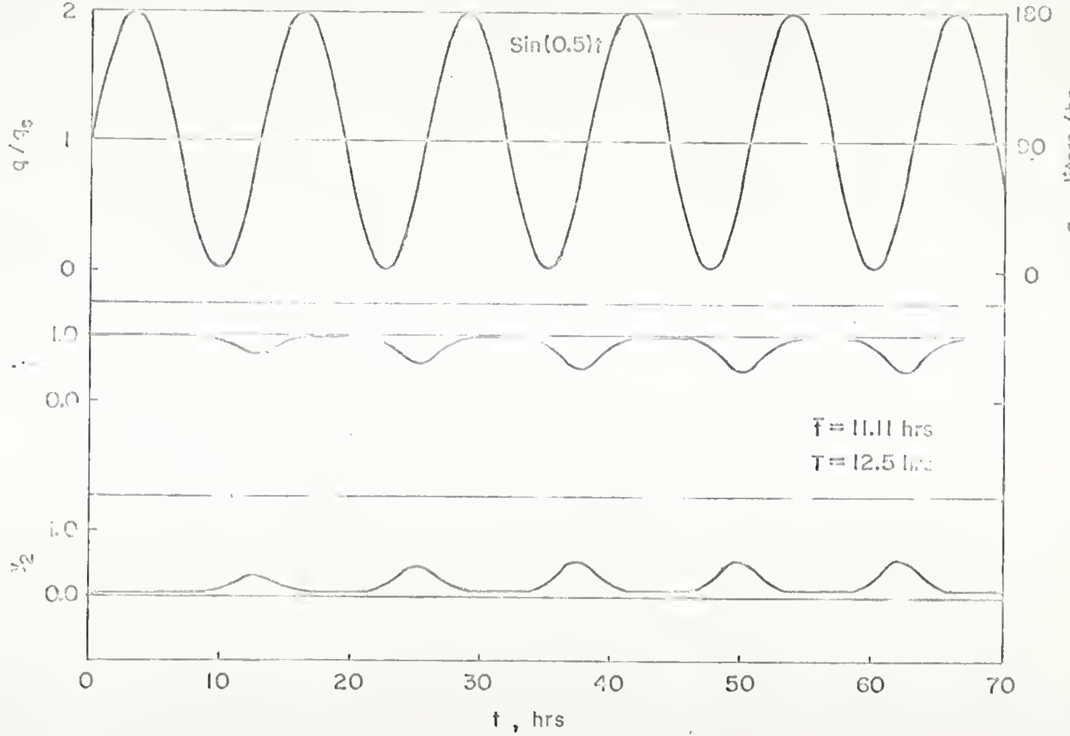

Fig. 30. Response of the system to a sinusoidal variation in the flow rate for $A_2 = 1$ and $W_2 = 0.5$.

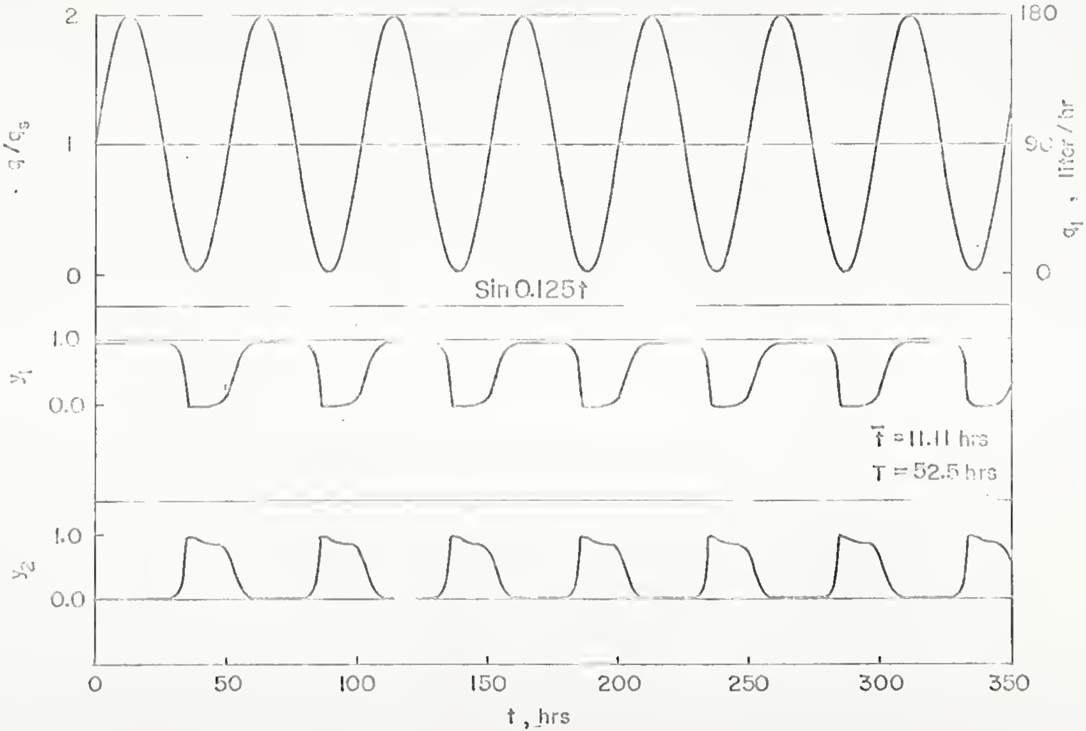

Fig. 31. Response of the system to a sinusoidal variation in the flow rate for $A_2 = 1$ and $w_2 = 0.125$.

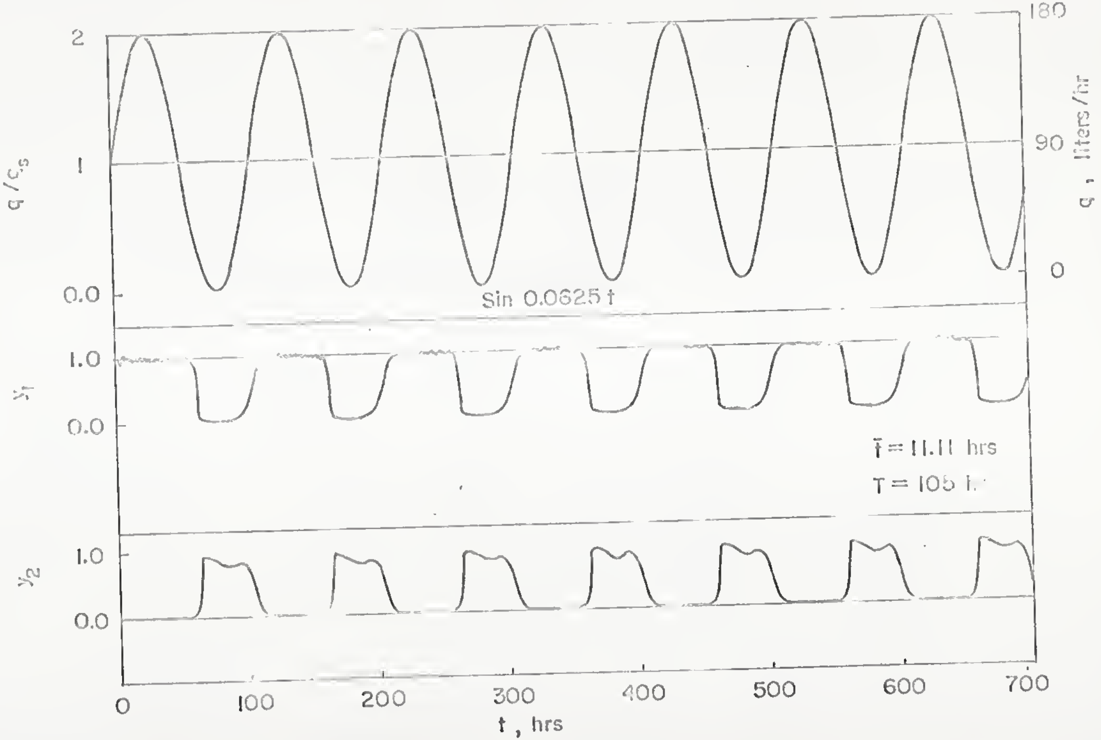

Fig. 32. Response of the system to a sinusoidal variation in the flow rate for $A_2 = 1$ and $W_2 = 0.0625$.

cyclic operation (34).

5. RESPONSE OF THE SYSTEM TO SIMULTANEOUS DISTURBANCES IN THE INFLUENT ORGANIC CONCENTRATION AND THE FLOW RATE

a. Performance Equations

In this section, response of the system to simultaneous sinusoidal variations of tha influent organic concentration, x_1^0, and the influent flow rata, q, is examined. Equations (50) and (51) represent the case where the steady state influent organic concentration is disturbed sinusoidally while the steady state flow rate remains constant. Equations (59) and (60) represent the case where the steady state influent organic concentration is disturbed sinusoidally while the steady state flow rate remains constant. Hence, the combination of these four equations should give rise to the performance equation for this case as shown below.

$$\frac{dy_1}{dt} \quad \frac{(1 + A_1 \sin \omega_1 t)}{\bar{t}_s} (1 + A_2 \sin \omega_2 t) - \frac{(1 + A_2 \sin \omega_2 t)}{\bar{t}_s} y_1$$

$$-(\frac{T}{\bar{t}})(\frac{y_1 \, y_2}{K_1 + y_1}) \tag{63}$$

and

$$\frac{dy_2}{dt} \quad \frac{(1 + A_2 \sin \omega_2 t)}{\bar{t}_s} y_2^0 - \frac{(1 + A_2 \sin \omega_2 t)}{\bar{t}_s} y_2 + (\frac{T}{\bar{t}})(\frac{y_1 y_2}{K_1 + y_1})$$

$$-(\frac{T}{t})(K_2 y_2) \tag{64}$$

respectively. In the above equations the dimensionless variables and parameters are defined as

$$y_1 = \frac{x_1}{x_{1s}^0}, \qquad y_2 = \frac{x_2}{Yx_{1s}^0}$$

$$y_1^0 = \frac{x_1^0}{x_{1s}^0}, \qquad y_2^0 = 0$$

$$K_1 = \frac{K}{x_{1s}^0} \qquad K_2 = \frac{k_D}{K}$$

$$\frac{x_1^0}{x_{1s}^0} = 1 + A_1 \sin \omega_1 t, \qquad \frac{q}{q_s} = 1 + A_2 \sin \omega_2 t$$

$$\tau = k\,\bar{t}$$

and the (steady state) mean holding time is defined as

$$\bar{t}_s = \frac{V}{q_x}, \text{ hr.}$$

b. Scaling and Static Test for the Analog Computer

The magnitude scaling for the system variable remains the same as it was in the preceding three sections. Hence, one can get scaled performance equations as

$$\frac{d[\frac{y_2}{2}]}{dt} = 2\left(\frac{1}{\beta\bar{t}_s}\right) \left[\frac{1 + A_1 \sin \omega_1 t}{2}\right] \left[\frac{1 + A_2 \sin \omega_2 t}{2}\right]$$

$$-2\left(\frac{1}{\beta \bar{t}_s}\right)\left[\frac{1+A_2\sin\omega_2 t}{2}\right]\left[\frac{y_1}{2}\right] \tag{65}$$

$$-\left(\frac{\tau}{\beta\bar{t}}\right)\frac{\left[\frac{y_1}{2}\right]\left[\frac{y_2}{2}\right]}{\left[\frac{K_1+y_1}{2}\right]}$$

and

$$\frac{d\left[\frac{y_2}{2}\right]}{dt}=\left(\frac{1}{\beta\bar{t}_s}\right)\left[\frac{(1+A_2\sin\omega_2 t)}{2}\right]y_2^0-2\left(\frac{1}{\beta\bar{t}_s}\right)\left[\frac{1+A_2\sin\omega_2 t}{2}\right]\left[\frac{y_2}{2}\right]$$

$$+\left(\frac{\tau}{\beta\bar{t}}\right)\frac{\left[\frac{y_1}{2}\right]\left[\frac{y_2}{1}\right]}{\left[\frac{K_1+y_1}{2}\right]}-\left(\frac{K_2\tau}{\beta\bar{t}}\right)\left[\frac{y_2}{2}\right] \tag{66}$$

respectively.

The scaled analog diagram for the analog computation is shown in Figure 33.

c. Results and Discussion

Figures 34 through 52 show the response of the system to the simultaneous sinusoidal variations of the influent flow rate, q, and the influent organic concentration, x_1^0. It is assumed that in each case the system originally operated at a steady state condition near the washout flow rate prior to the applications of disturbances. The steady state value of the influent organic concentration, x_{1s}^0, is 200 mg/liters and the steady state influent flow rate is 90 liters/hr, and the corresponding mean holding time is 11.1 hrs. Once again, the flow rate near the washout condition is selected because it is a critical condition of the system which is of considerable practical significance.

In Figures 34 through 37 the fluctuation of q is 20%, that is, the flow rate oscillates between 72 and 108 liters/hr., and the fluctuation of x_1^0 is 100%, which represents an oscillation between 0 and 400 mg/liter. With these amplitudes of oscillation, the frequencies of oscillations of both q and x_1^0 are varied in the same manner simultaneously between values of 5.0 radian/hr to 0.0625 radian/hr. It is observed that disturbances have little or no effect on the organism concentration, y_2. This should be expected because when the disturbances in x_1^0 and q are applied individually at high frequency of oscillation, y_2 is hardly affected (see Figures 20 and 25). However, the organic concentration, y_1, is observed to vary appreciably. This variation is due to the fluctuation of x_1^0 rather than that of the q. It has been observed that when the fluctuation in x_1^0 is large, y_1 also fluctuates appreciably at any frequency when q is constant (see Figures 20 through 23).

It is also observed in Figures 34 through 37 that the mean concentration values under the cyclic steady state condition are only slightly different from the original steady state values of the system.

In the next four figures (Figures 38 through 41), the amplitude of the fluctuation of q is 100%, and that of x_1^0 is 20%. With these amplitudes of oscillation, the frequencies of oscillations of both q and x_1^0 are varied in the same manner as is done in the case of Figures 34 through 37. In contrast to Figures 34 through 37, the responses for the organic and organism concentrations in Figures 38 through 41 definitely reveal the non-linearity of the system except when the

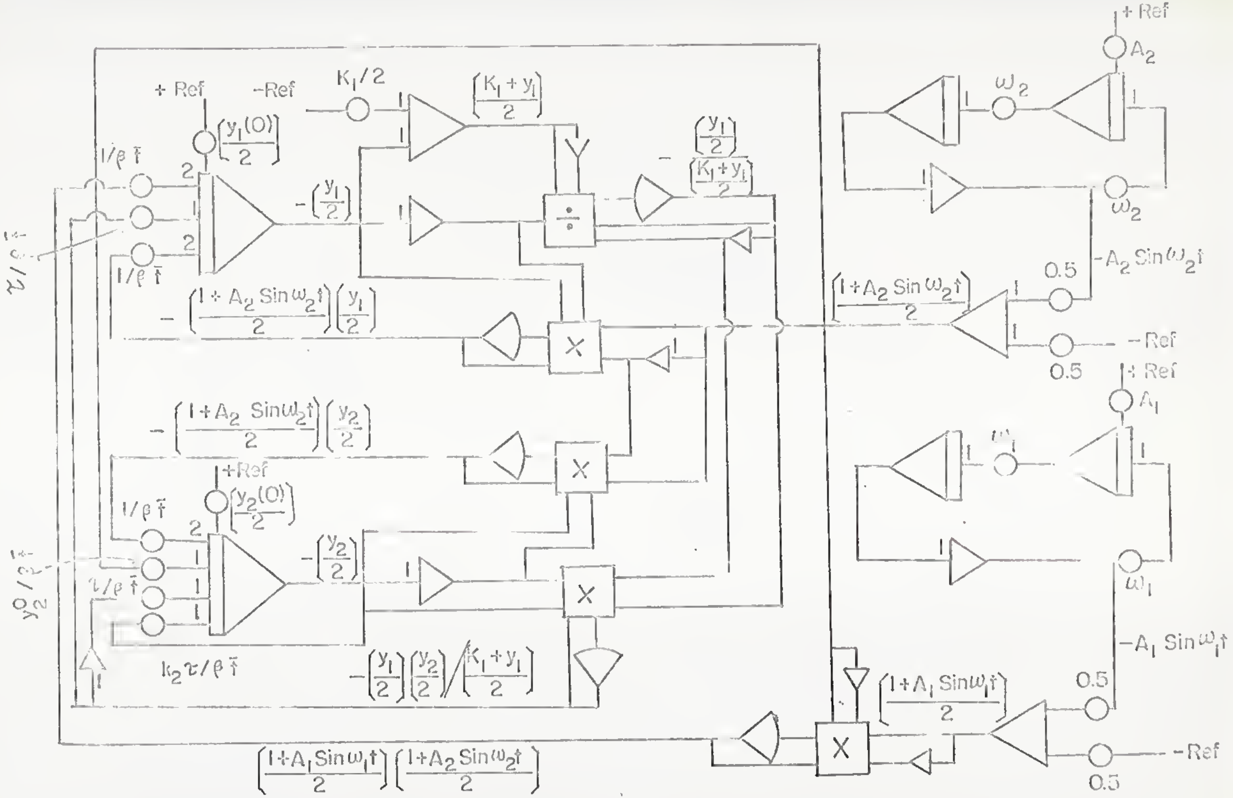

Fig. 33. Scaled diagram for equations (65) and (66).

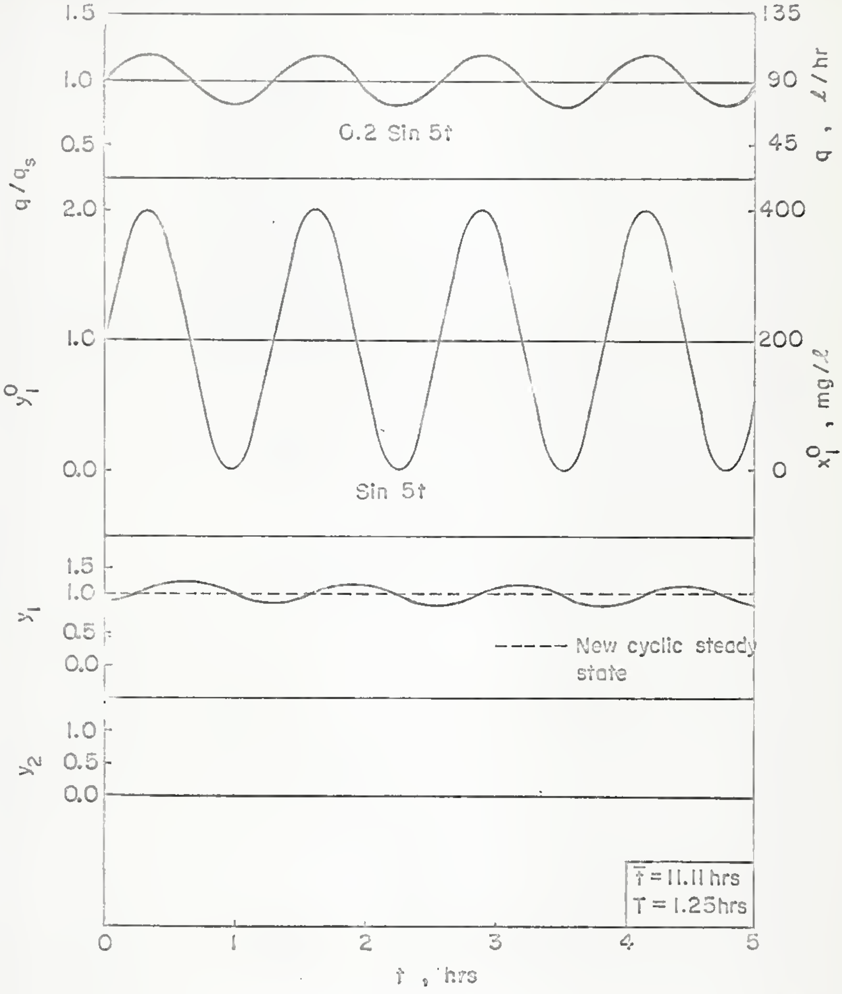

Fig. 34. Response of the system to a simultaneous sinusoidal variations in the q and x for $A_1 = 1$, $A_2 = 0.2$ and $\omega_1 = \omega_2 = 0.5$.

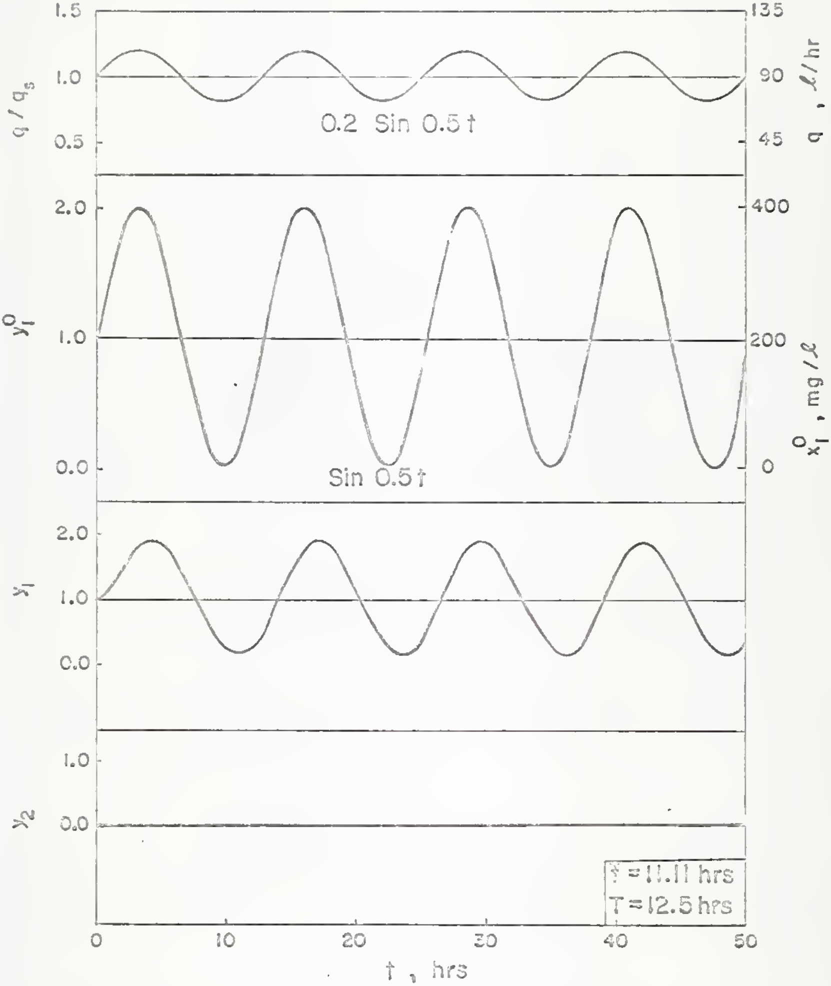

Fig. 35. Response of the system to a simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = 1$, $A_2 = 0.2$ and $\omega_1 = \omega_2 = 0.125$.

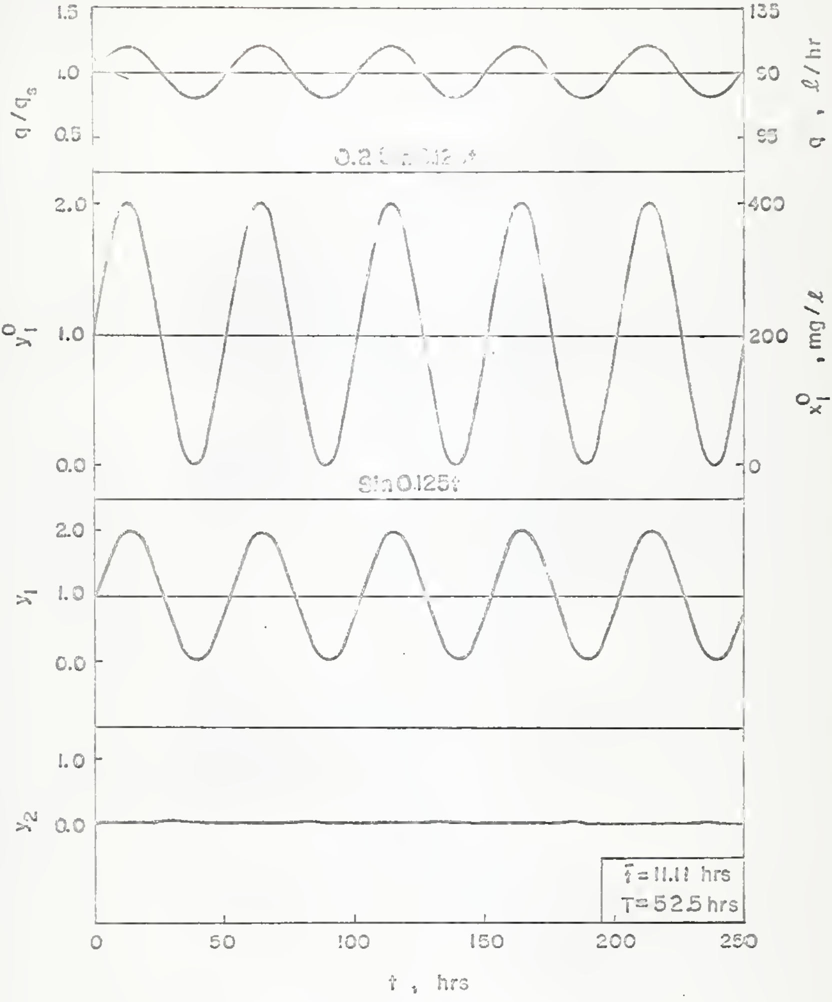

Fig. 36. Response of the system to a simultaneous sinusoidal variations in the q and x for $A_1 = 1$, $A_2 = 2$ and $\omega_1 = \omega_2 = 0.125$.

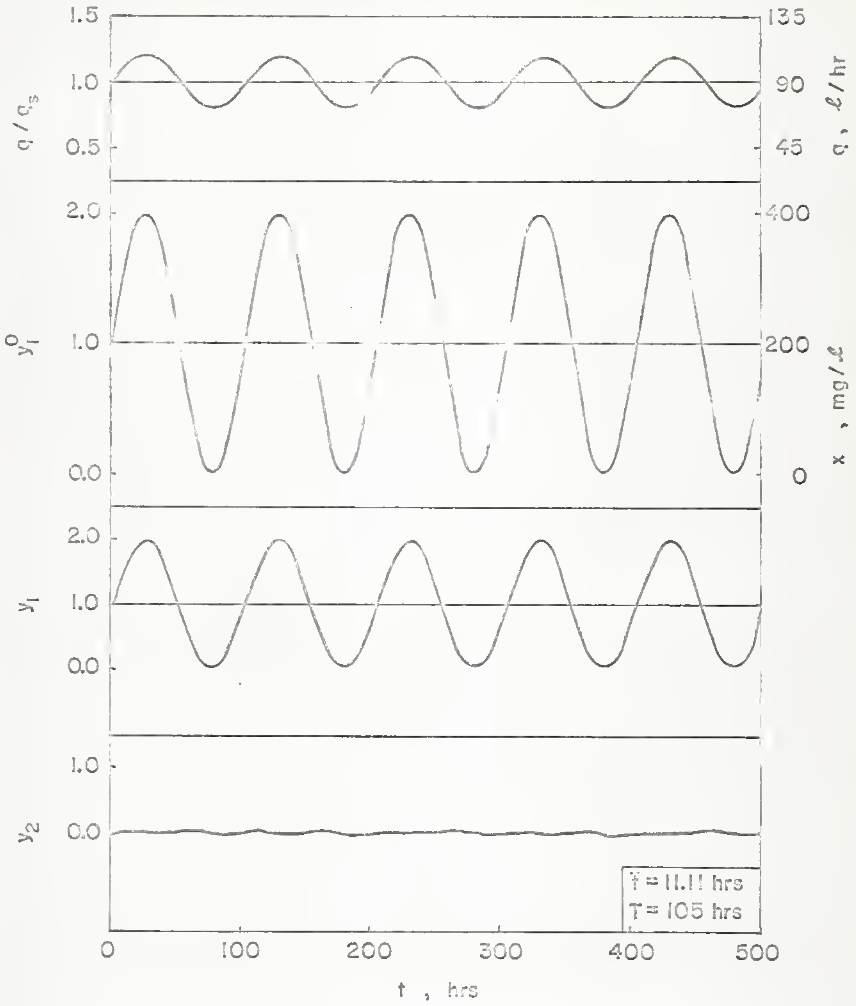

Fig. 37. Response of the system to a simultaneous sinsoidal variations in the q and x_1^0 for $A_1 = 1$, $A_2 = 0.2$ and $\omega_1 = \omega_2 = 0.0625$.

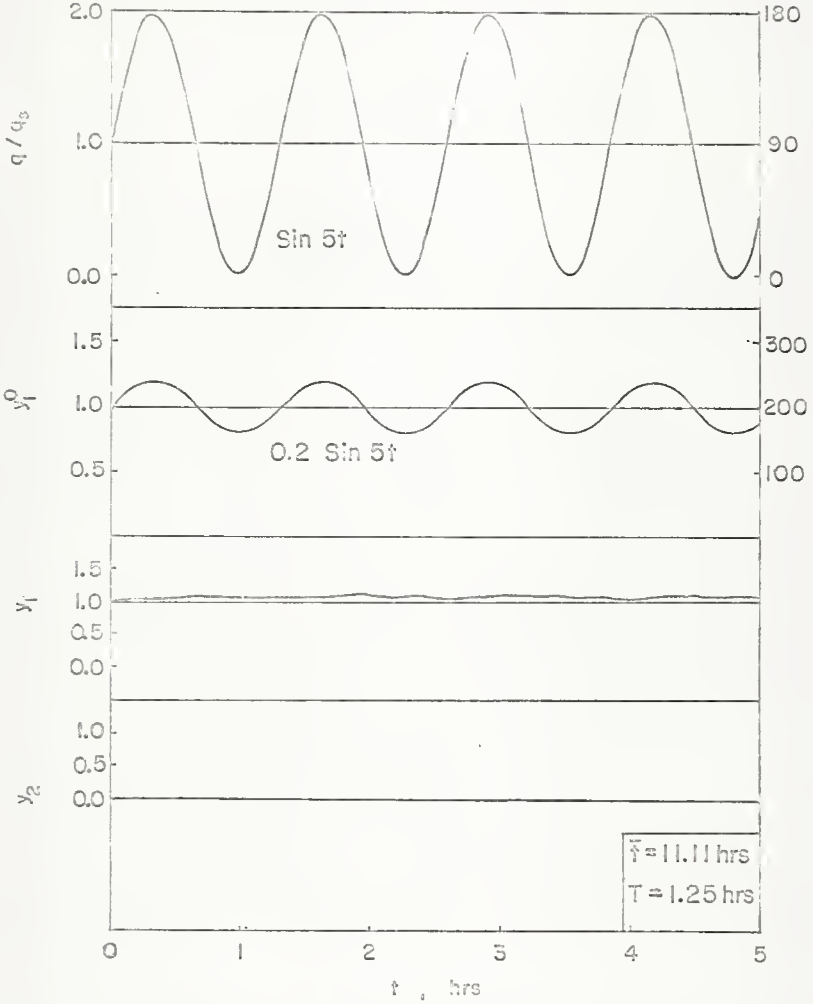

Fig. 38 . Response of the system to a simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = 0.2$, $A_2 = 1$ and $\omega_1 = \omega_2 = 5$.

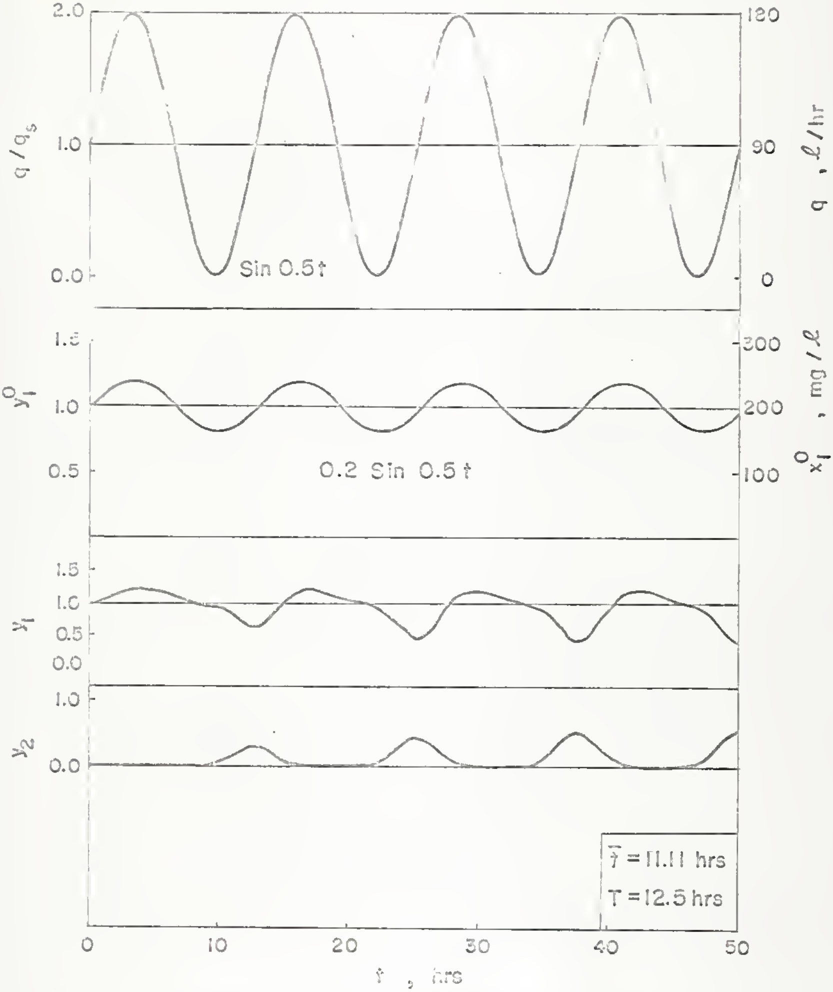

Fig. 39. Response of the syst[illegible] simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = 0.2$, $A_2 = 1.0$ and $\omega_1 = \omega_2 = 0.5$.

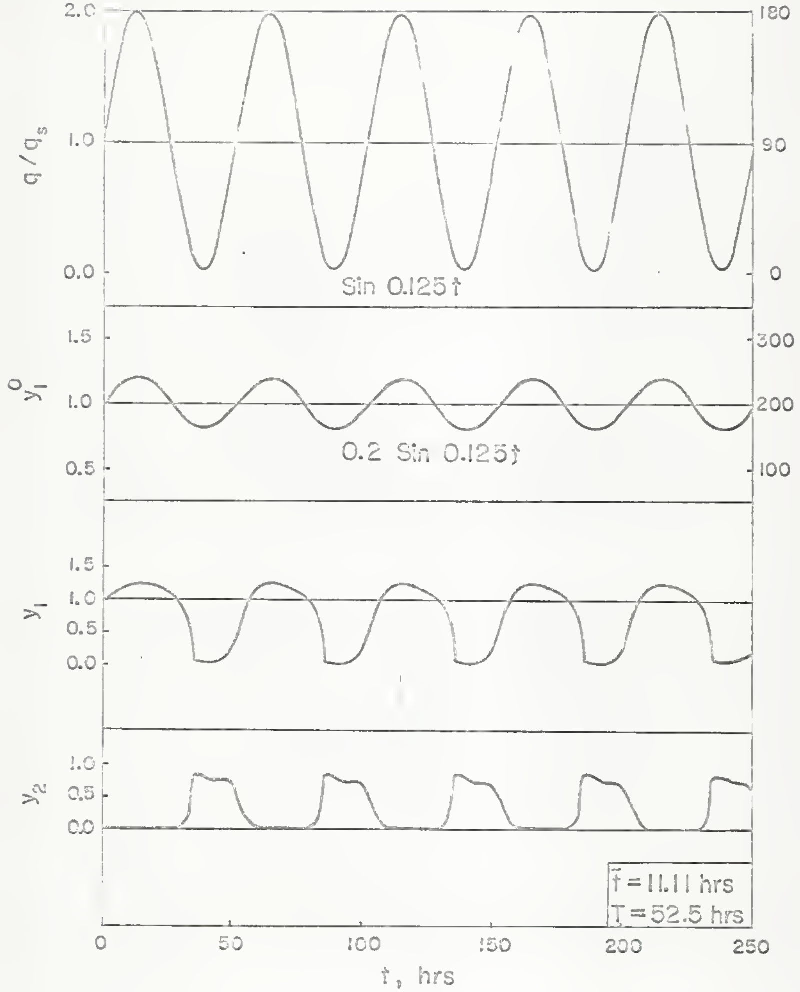

Fig. 40. Response of the system to a simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = 0.2$, $A_2 = 1$ and $\omega_1 = \omega_2 = 0.125$.

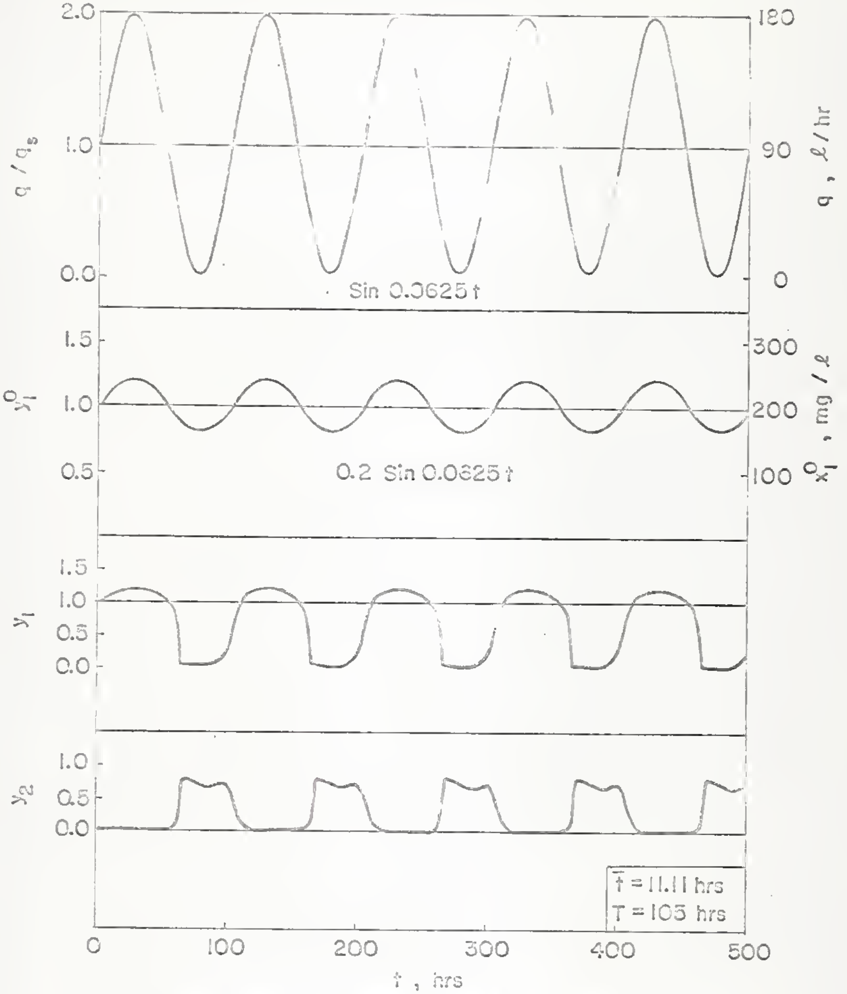

Fig. 41. Response of the system to a simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = 0.2$, $A_2 = 1.0$, and $\omega_1 = \omega_2 = 0.0625$.

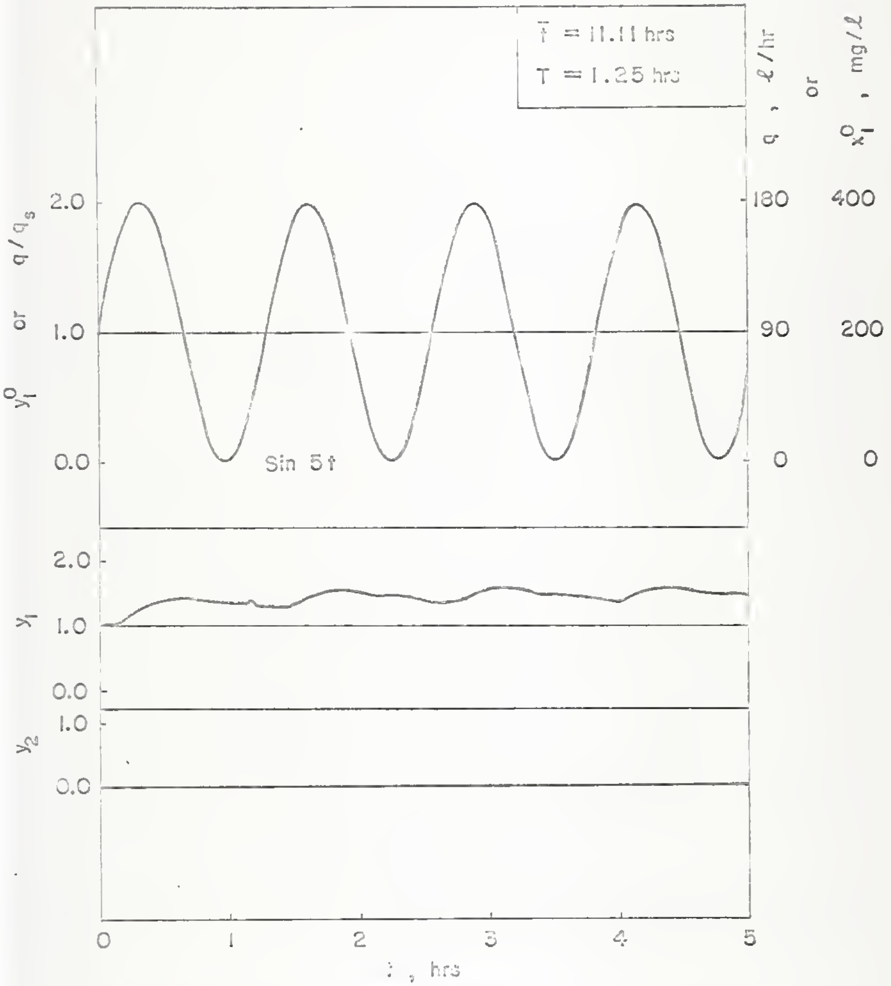

Fig. 4.2. Response of the system to a simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = A_2 = 1$ and $\omega_1 = \omega_2 = 5$.

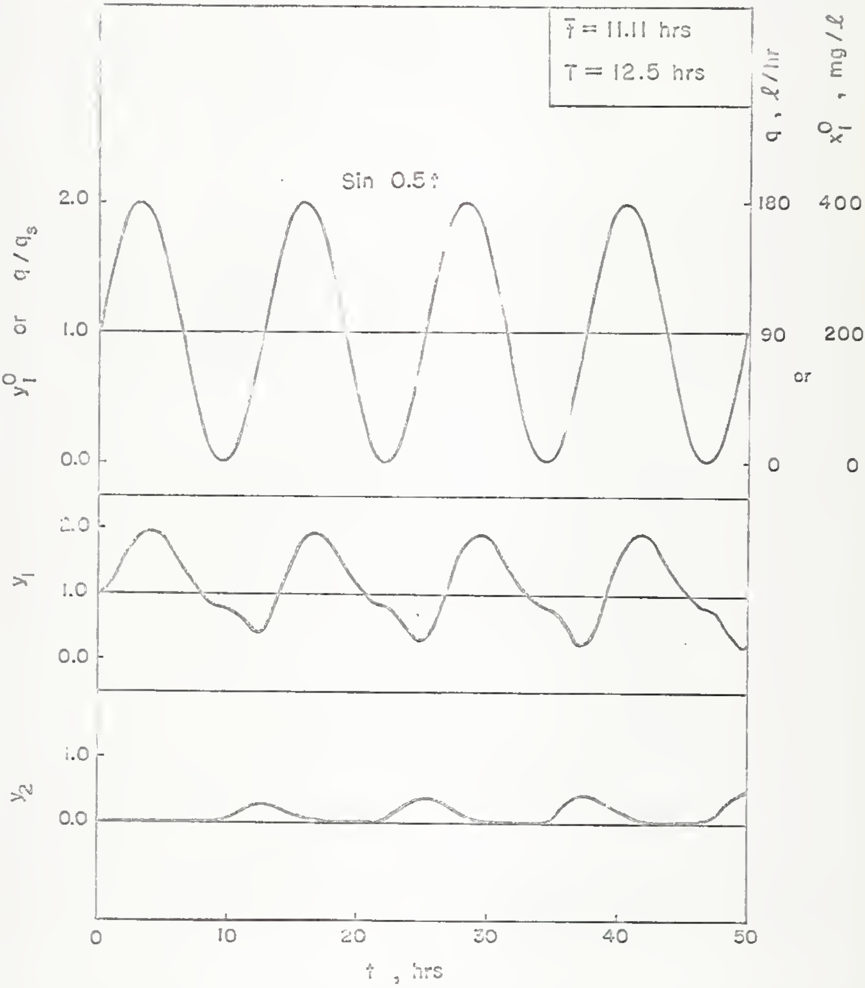

Fig. 43. Response of the system to a simultaneous sinusoidal variations in the q and x_1^o for $A_1 = A_2 = 1$ and $\omega_1 = \omega_2 = 0.5$.

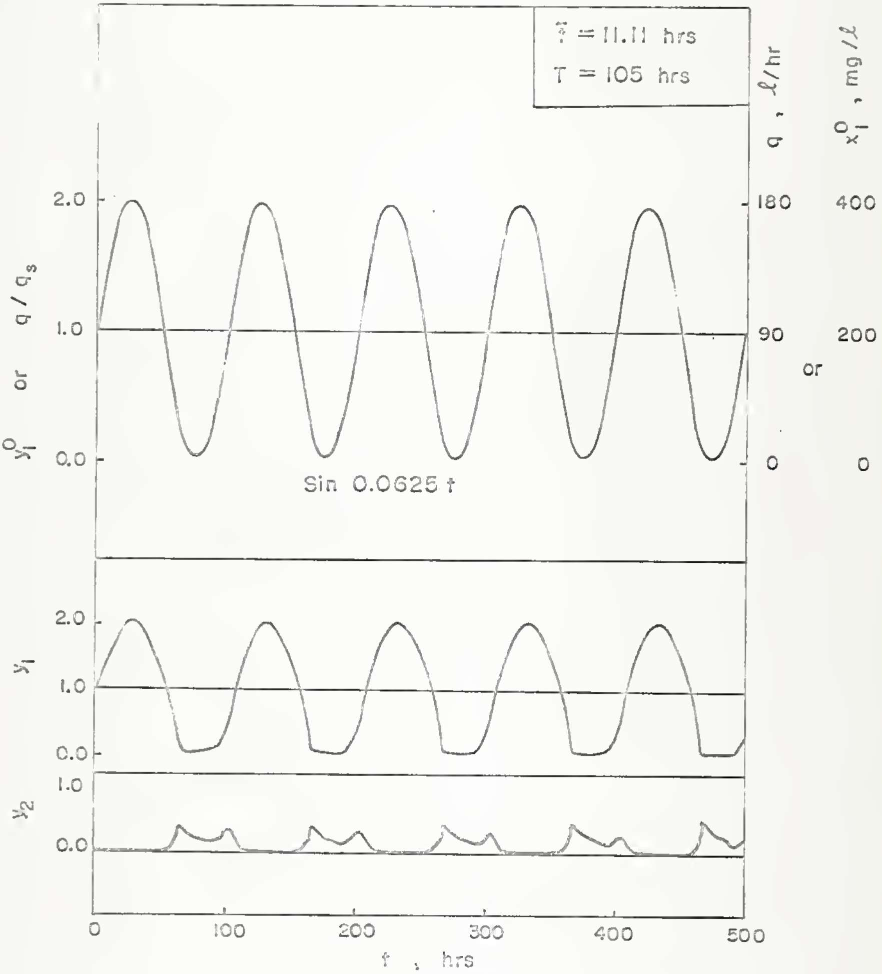

Fig. 44. Response of the system to a simultaneous sinusoidal variations in the q and x for $A_1 = A_2 = 1$ and $\omega_1 = \omega_2 = 0.0625$.

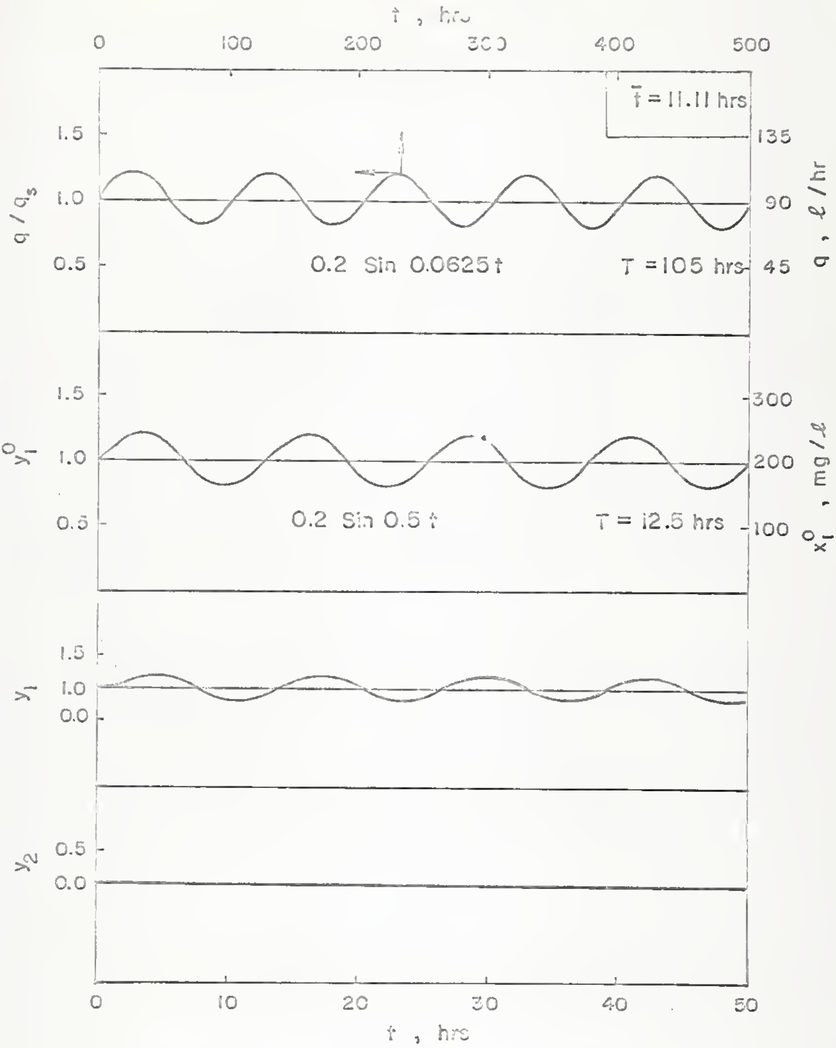

Fig. 45. Response of the system to a simultaneous sinusoidal variations in the q and x for $A_1 = A_2 = 0.2$ $\omega_1 = 0.5$ and $\omega_2 = 0.0625$.

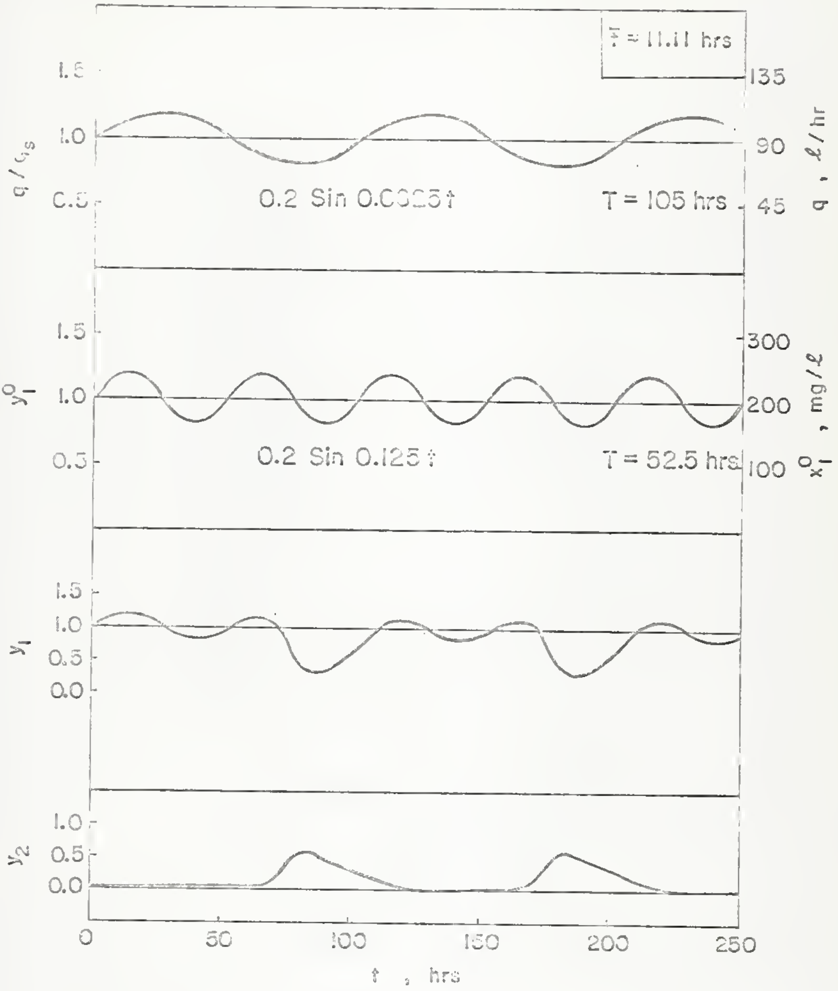

Fig. 46. Response of the system to a simultaneous sinusoidal variations in the q and x_1^o for $A_1 = A_2 = 0.2$, $\omega_1 = 0.125$ and $\omega_2 = 0.0625$.

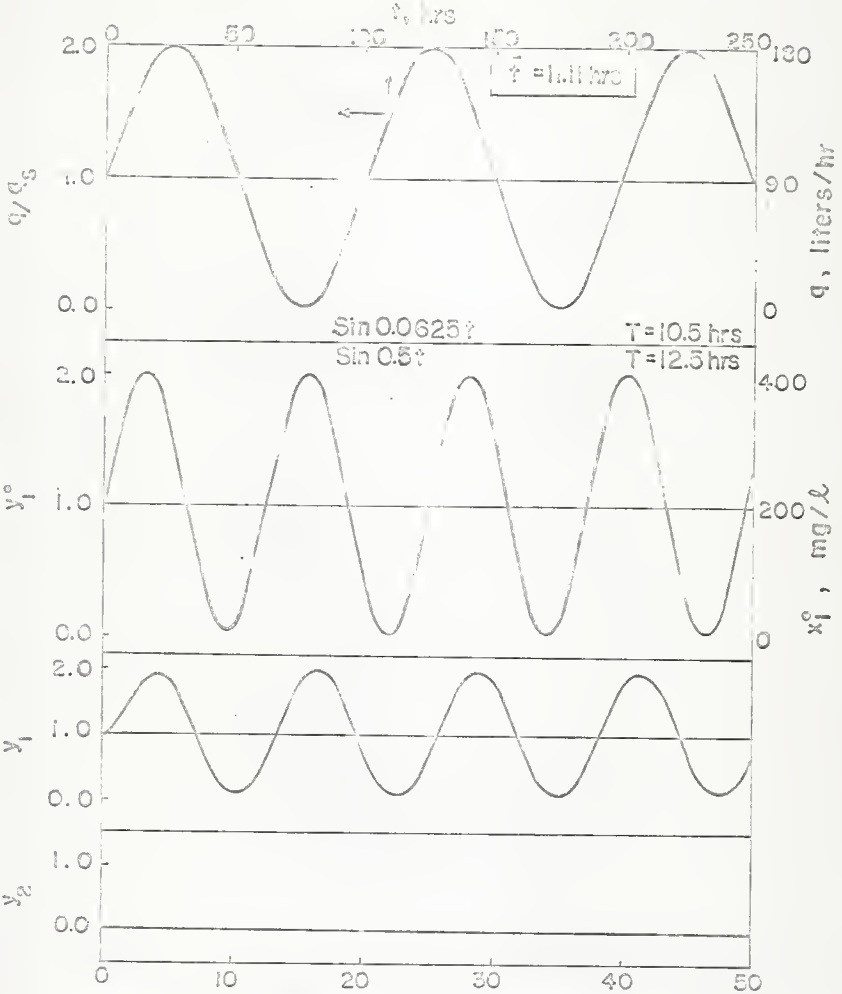

Fig.47. Response of the system to a simultaneous sinusoidal variations in the q and x_1^o for $A_1=A_2=1$, $\omega_1=0.5$ and $\omega_2=0.0625$.

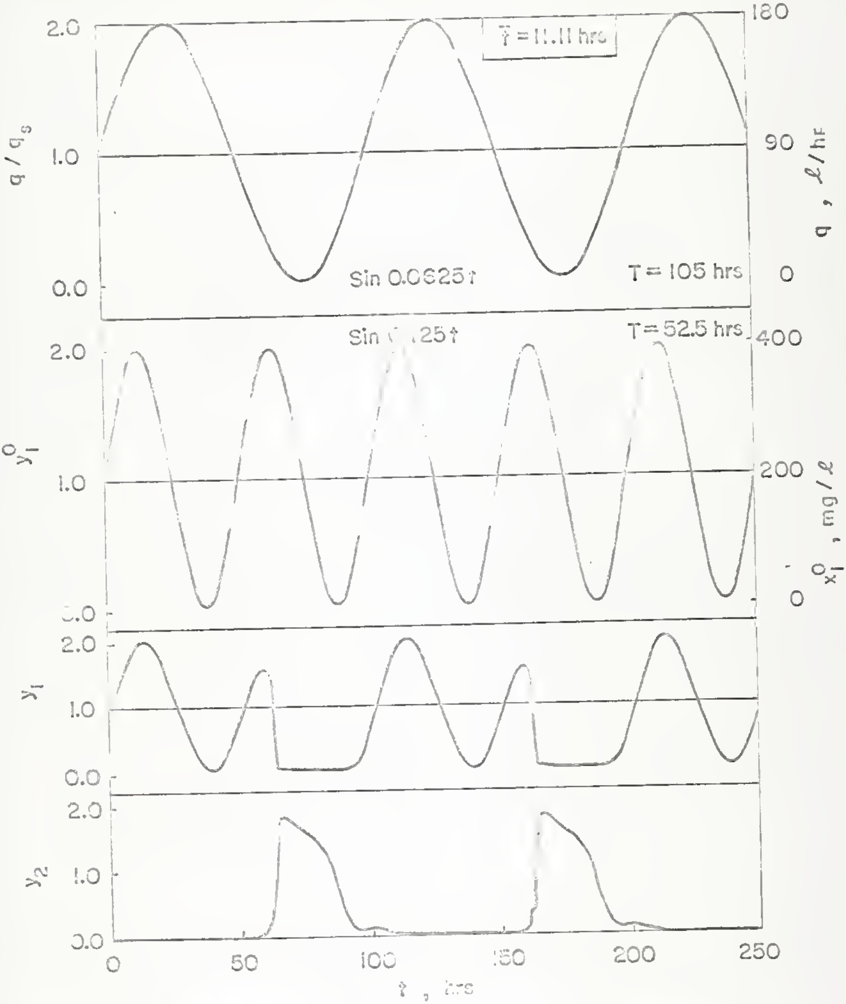

Fig. [illegible] Responses [illegible] to a simultaneous sinusoidal variation in the q and x_1^0 for $A_1 = A_2 = 1$, $\omega_1 = 0.125$ and $\omega_2 = 0.0625$.

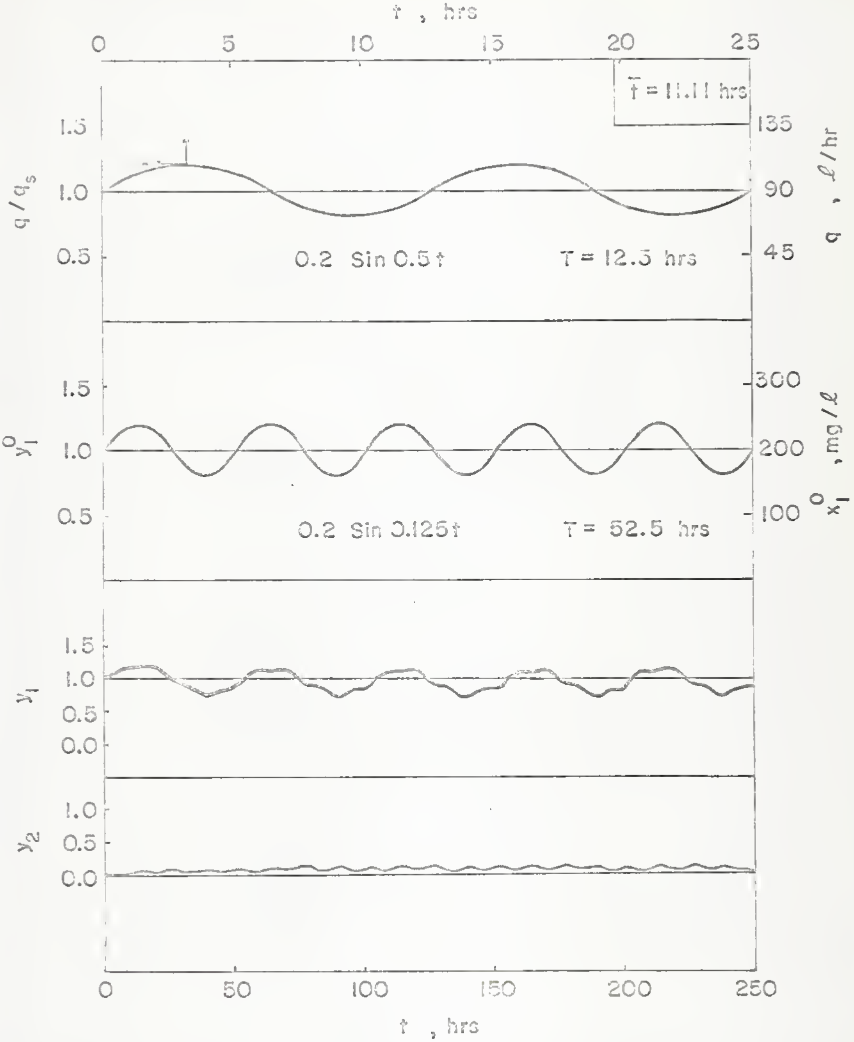

Fig. 49. Response of the system to a simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = A_2 = 0.2$, $\omega_1 = 0.125$ and $\omega_2 = 0.5$.

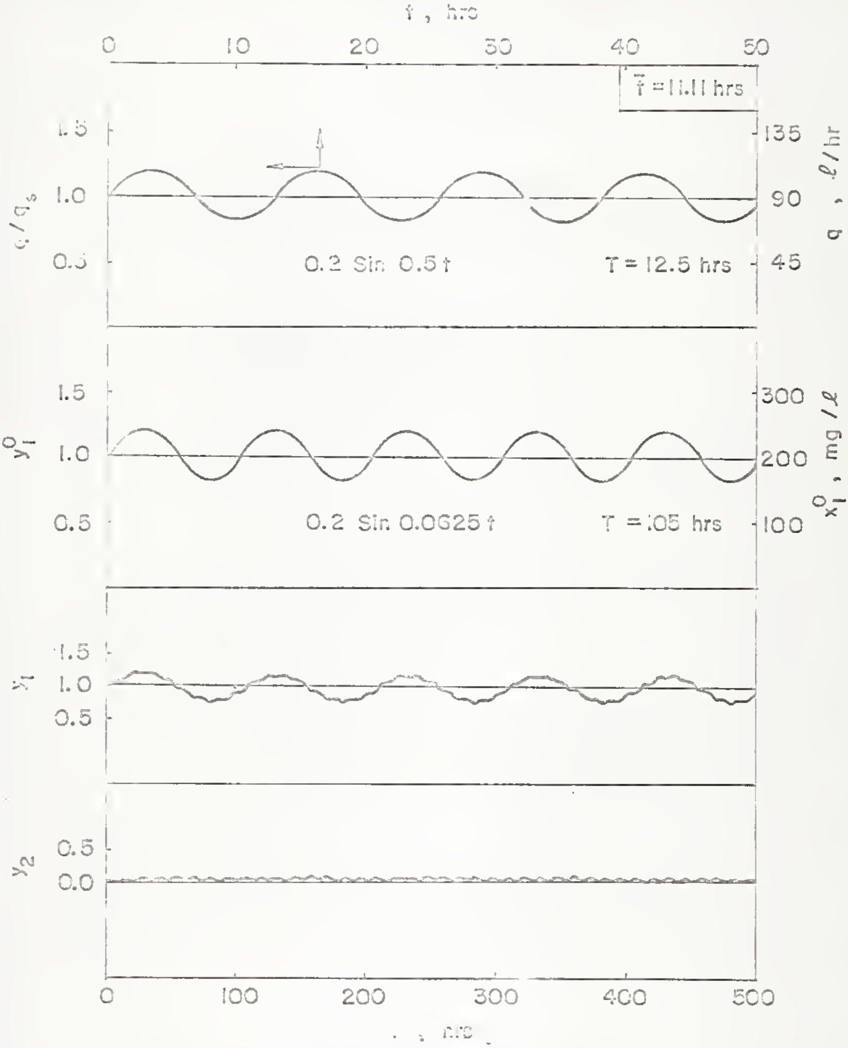

Fig. 5C. Response of the system to a simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = A_2 = 0.2$, $\omega_1 = 0.0625$ and $\omega_2 = 0.5$.

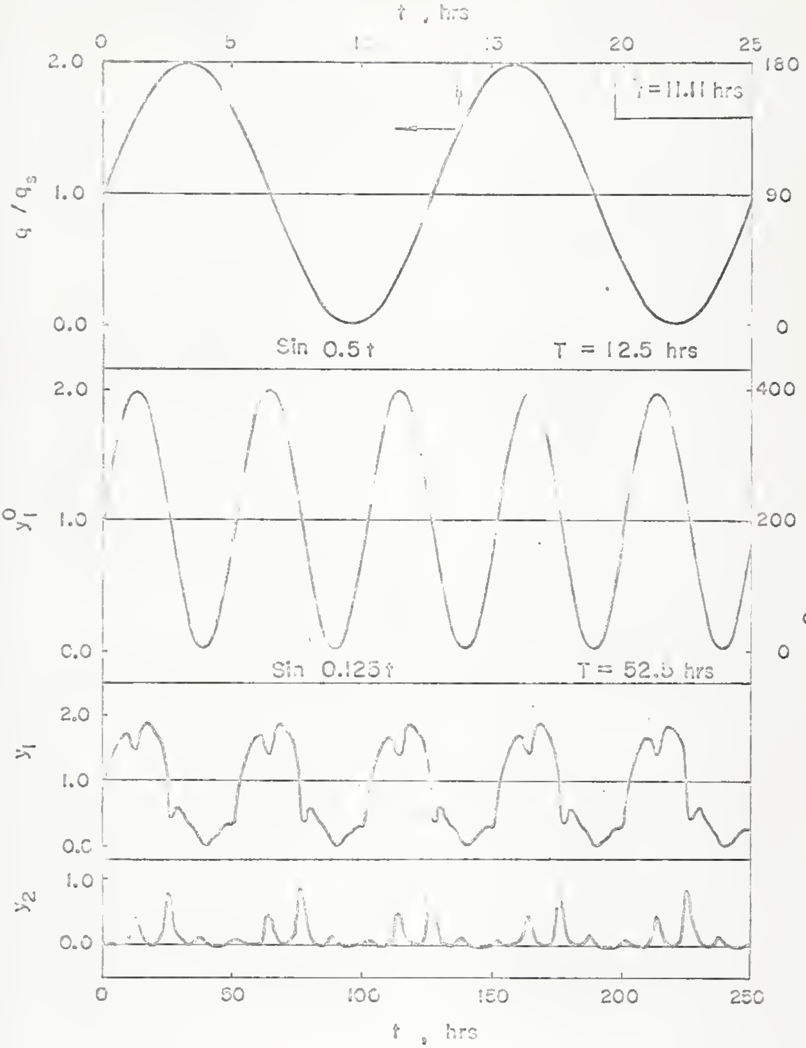

Fig. 51. Response of the system to simultaneous sinusoidal variations in the q and x_1^0 for $A_1 = A_2 = 1$, $\omega_1 = 0.125$ and $\omega_2 = 0.5$.

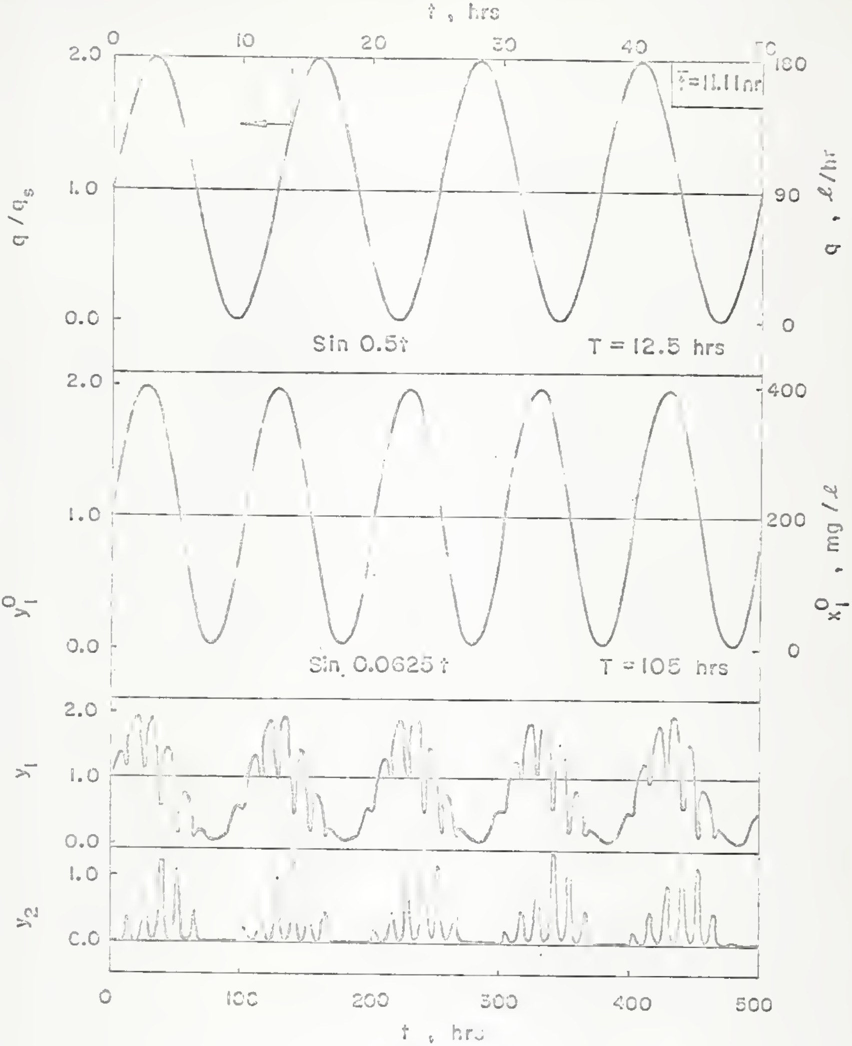

Fig. 52. Response of n[illegible] [illegible] simultaneous sinusoidal variations in [illegible] q and x_1^0 for $A_1 = A_2 = 1$, $\omega_1 = 0.0625$ and $\omega_2 = 0.5$.

frequency of oscillation is extremely high. Appearance of the non-linearity is mainly due to the large amplitude of the fluctuation in q. Note that a similar observation has been made in the preceeding section when only the fluctuation in q is applied to the system, (see Figures 30, 31 and 32). In general, it is observed that the simultaneous sinusoidal variation of q and x_1^0, as stated above improves the performance of the system near the washout condition, since the mean average values of the concentrations change to new and more favorable cyclic steady state values.

In Figures 42 through 44 the dimensionless amplitude and frequencies of the fluctuations of q and x_1^0 are identical. That is, dimensionless amplitudes of A_1 and A_2 are one, and they represent a range of x_1^0 between 0 and 400 mg/liter and a range of q between 0 and 180 liters/hr respectively. The frequency of fluctuation is varied within the ranges corresponding to that between a tenth of the mean holding time to approximately ten times the mean holding time. Figure 42 shows the system's response at a very high frequency of oscillation. The organic concentration response curve shows a non-linearity. It should be noted, however, that the organism response still remains unchanged. For a period of oscillation ten times larger than the mean holding time, the non-linearity of the system is apparent as shown in Figure 44.

Figures 45 and 46 show the system responses for cases where the amplitudes of the disturbances of q and x_1^0 are both 20% but where the period of oscillation of q is ten times larger than the mean holding time of the system (that is, the frequency of oscillation is very small) and the period of oscillation of x_1^0 is varied from that equal to the mean holding time to approximately five times the mean holding time. Thus, the frequency of the influent flow rate disturbance is always smaller than that of the influent organic concentration.

It is observed that at a very high frequency of oscillation of x_1^0 compared to the frequency of oscillation of q, there is little effect on the organism concentration as seen from Figure 45. In Figure 45, the organic response curve shows no non-linearity effect but shows the fluctuation, and a cyclic steady state value of the organic concentration remains near the original steady state value. As before, at lower frequencies of oscillations of q and x_1^0 (see Figure 46), the non-linearity of the system becomes apparent. Figures 47 and 48 are similar to Figures 45 and 46, but in Figures 47 and 48 the amplitudes of the fluctuations of x_1^0 and q are both 100% instead of 20%. The same range is used as in Figures 45 and 46 for the periods of oscillation. The results are similar to those observed in Figures 45 and 46 but show a higher degree of non-linearity of the system at lower frequencies of oscillation.

Figures 49 and 50 represent the cases where the amplitudes of disturbances of q and x_1^0 are identical at 20%, but where the period of oscillation of q is the same as the mean holding time of the system (that is, the frequency of oscillation is fairly high) and the period of oscillation of x_1^0 is varied approximately from five times the mean holding time to ten times the mean holding time. Thus, the frequency of influent flow rate disturbance is always larger than that of the influent organic concentration. It is observed in Figures 49 and 50 that the organism concentration attains a new cyclic steady state value which is higher than the original steady state value of the organism concentration. Similarly the organic concentration attains a lower cyclic steady state value than its original steady state value. Hence, once again it is observed that the simultaneous sinusoidal variations of q and x_1^0 improve the performance of the system near the washout condition. However, Figures 51 and 52 are similar to Figures 49 and 50, but the amplitudes of fluctuations of x_1^0 and q are both 100% instead of 20%. It is observed in Figures 51 and 52 that the response of the system is highly non-linear and fairly irregular for a given period of oscillation. This irregularity occurs because of a superimposition of a higher frequency of oscillation of q on the lower frequency of oscillation of x_1^0.

In general, in these figures it is observed that simultaneous sinusoidal variation of q and x_1^0 improve the performance of the system near the washout condition, since the original near washout steady state values chang to new, more favorable cyclic steady state values. It is also observed that systems show nonlinearity at very low frequency of oscillation of q and x_1^0. The system also becomes oscillatory when a higher frequency of oscillation of q is superimposed on a lower frequency of oscillation of x_1^0. In the same way the irregular response of the system is observed in a given period of oscillation.

Chapter V

CONCLUSION

In the second part of this work a mathematical model for the continuously operated bioreactor system which can be used to represent a biological waste water treatment process has been developed. Analyses of steady state and critical conditions of the process have also been investigated fully. Dynamic characteristics of this model system under various operating conditions have been simulated on a desk top analog computer, EAI TR-48.

The transient response of the system under the constant influent flow rate and constant influent organic concentration is observed during the plant start-up or restart-up period. Responses of the system to step changes in the influent flow rate are also examined. It has been observed that theoretically the one stage isothermal continuous stirred tank reactor system never does completely attain the condition of washout from the normal operating condition.

Responses of the system to the sinusoidal variations of the influent organic concentration are also observed. It can generally be concluded that a very high fluctuation in influent organic concentration reduces the capacity of the plant.

Responses of the system to the sinusoidal variations of the influent flow rate are also examined. In general, the cyclic variation in the influent flow rate improves the performance of the system near the washout condition especially when the period of fluctuation is large.

The responses of the system to simultaneous variations in q and x_1^0 are also examined. The simultaneous variations in q and x_1^0 also improve the performance of the system. Very irregular and random like responses of the system are often observed when the two fluctuations are superimposed on each other.

It is also observed, in general, that very high frequencies of disturbances (or very small periods of oscillations) have little or no effect on the system; that is, the system remains near the original steady state condition. The non-linearity of the system is observed for very low frequencies of disturbances which correspond to very high periods of oscillations of disturbances.

NOMENCLATURE

SYMBOLS

x_1^n	concentration of organics in the outlet stream of nth stage, mg/liter
x_2^n	concentration of organisms in the outlet stream of nth stage, mg/liter
x_1^0	influent organic concentration, mg/liter
x_2^0	influent organism concentration, mg/liter
x_1	concentration of organics in the outlet stream of the 1st stage, mg/liter
x_2	concentration of organisms in the outlet stream of the 1st stage, mg/liter
μ	growth rate constant, hr^{-1}
k	specific reactor rate constant which is equivalent to the maximum growth rate when the organic concentration is not limiting the rate q growth, hr^{-1}
k_D	the specific endogeneous microbial attriation rate, hr^{-1}
r	growth rate, mg/liter, hr
K	parameter (a constant) in a kinetic model which is equivalent to the concentration g organics at which the specific growth rate observed is one half the maximum value; saturation constant, mg/liter
Y	yield factor mg/mg
q	volumetric flow rate
V^n	volume of nth stage liters
$\bar{t}^n$	nominal holding time for nth stage
$\bar{\tau}^n_{wm}$	minimum mean holding time corresponding to the washout condition of $y_1^n \to 1,\ y_2^n \to 0$ for nth stage, hr
$\bar{\tau}^n_{qm}$	minimum mean holding time corresponding to the washout condition of $y_1^n \to \infty,\ y_2^n \to -\infty$ for nth stage, hr

y_1^n	dimensionless organic concentration in the outlet stream of nth stage
y_2^n	dimensionless organism concentration in the outlet stream of nth stage
K_1	dimensionless organic concentration at which the specific growth rate observed is one half the maximum value
K_2	dimensionless endogeneous respiration rate
τ^n	dimensionless mean holding time
y_{1s}^n	dimensionless steady-state organic concentration
y_{2s}^n	dimensionless steady-state organism concentration
x_{1s}^0	steady-state influent organic concentration, mg/liter
q_s	steady-state flow rate, liters/hr
$\bar{t}_s$	steady-state mean holding time, hr
A	amplitude of the sinusoidal disturbance in the influent organic concentration, mg/liter
B	amplitude of the sinusoidal disturbance in the flow rate, liters/hr
A_1	dimensionless amplitude of the sinusoidal variations in the influent organic concentration
A_2	dimensionless amplitude of the sinusoidal variations in the flow rate
ω_1	angular frequency of the sinusoidal variations in the steady state influent organic concentration, radian/hr
ω_2	angular frequency of the sinusoidal variations in the flow rate, radian/hr
f_1	cyclic frequency of the sinusoidal variations in the steady state influent organic concentration, cycles/hr
f_2	cyclic frequency of the sinusoidal variation in the steady state flow rate, cycles/hr

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CHEMICAL PROCESS ANALYSIS AND OPTIMIZATION USING AN ANALOG COMPUTER

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AN ABSTRACT OF A MASTER'S REPORT

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MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY
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ABSTRACT

In the first part of this work the behavior of the autocatalytic reactor system is studied on an analog computer. Specifically, the minimum mean holding time or the minimum volume of a particular system is found for the various conversions. It is well known that most biochemical reactors are autocatalytic; therefore, in the second part of this work a mathematical model for the continuously operated bioreactor system which can be used to represent a biological waste water treatment process is developed. Dynamic characteristics of this model system under various operating conditions have been simulated on a desk top analog computer, EAI TR-48. Four different cases have been considered. In the first case, the steady state influent flow rate of the system and steady state influent organic concentration are held constant and transient behavior of the system during the start-up or restart-up of the plant is observed. This also gives information on the responses of the system to a step change in the steady state flow rate. Phase-plane plots are also obtained by eliminating the independent time variable t and plotting one state variable against the other. In the second case, responses of the system to a sinusoidal variation of the influent organic concentration are examined. The steady state influent flow rate is assumed to remain constant throughout the process. In the third case, responses of the system to the sinusoidal variations of the influent flow rate are examined while the steady-state influent organic concentration is kept constant. In the fourth and final case, responses of the system to the simultaneous sinusoidal variations of the influent organic concentration and the influent flow rate are examined. It is observed, in general, that for very high frequencies of disturbances (or very small periods of oscillation), disturbances in the feed condition have little or no effect on the system, that is, the system mainly remains near the original steady state values. The non-linearity of the system shows up when frequencies of disturbancies are very low (or when periods of oscillation are very high). It is also observed that the sinusoidal variation of the influent flow rate improves the performance of the system near the washout condition especially when the period of disturbance is large. The steady state behavior and critical conditions of the system have also been investigated.