SIMULATION AND OPTIMIZATION OF A TWO STAGE CONTINUOUS ANAEROBIC DIGESTER SYSTEM

by 680

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I. INTRODUCTION

Biological processes have been operated as continuous flow systems for many years. However, development of mathematical models for such systems has been more recent (since 1950) with significant early contributions by Novick and Szilard (1), Monod (2), and Herbert (3). Most of the earlier work was devoted to the analysis of pure bacterial cultures in single-stage reactors.

More recently, there has been much interest in the analysis of biological waste water treatment (4,5,6). These works again assumed that the process involved a single culture.

However, anaerobic digestion is a complex process and in the recent past, growing attention has been given to it from both the theoretical and experimental points of view. Malina and McCarty (7,10) refer to anaerobic digestion as a complex two-step process involving various intermediate chemical species and several types of organisms. This mechanism is now widely used. Willimon and Andrews (9) carried out experimental work using a single stream system under various operating conditions. These authors (8) have given a mathematical formulation of the kinetic model of the anaerobic process which allows them to simulate one-stage and two stage processes. Finally, Pfeffer (13) has emphasized the advantages of a contact process (i. e. including recycle of organisms) as contrasted with a conventional system.

In this work a mathematical formulation employing the kinetic model of Willimon and Andrews is used to simulate conventional and contact anaerobic processes consisting of two stages. In addition, by adjoining an economic model to the process model, the process is optimized for various values of the recycle ratio.

The results obtained by this approach must be balanced with engineering judgment and experience. The kinetic and economic models can only approximate reality. Nevertheless, this study may yield a better understanding of the process and a more efficient industrial application.

II. BASIC RELATIONSHIPS

1. Mechanism of anaerobic fermentation (7)

The anaerobic treatment of waste water involves several microbial species which carry out numerous biochemical and microbiological reactions (see Figure 1). The process yields carbon dioxide CO_2, methane CH_4, and reduced organic molecules (H_2S, etc...). The bacterial population consists of facultative organisms which tolerate small amounts of dissolved oxygen and anaerobic bacteria.

The anaerobic fermentation process is a sequential one including two distinct steps, which are the "acid fermentation" step and the "methane fermentation" step. During the "acid fermentation" step, "acid producing bacteria" break complex organic compounds down to simpler organic structures, as bacterial growth takes place. The principal intermediate compounds resulting from "acid fermentation" are volatile acids, i.e. short-chain carboxylic acids (C_1 to C_6). These volatile acids provide substrate for

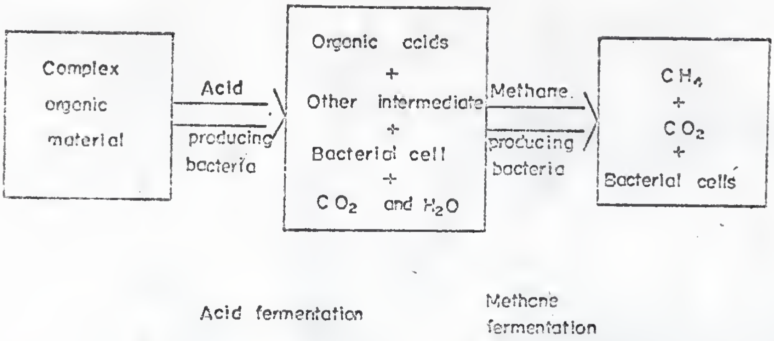


Fig. 1 Sequential mechanism of anaerobic waste treatment (7).

the "methane-froming" bacteria. During "methane fermentation", the organic acids produced during the "acid fermentation" step are converted into carbon dioxide and methane. These bacteria are substrate specific, i. e. each of these ferments only a small group of intermediate compounds. This fact has also been recognized by Willimon and Andrews (9) in their experimental work. Thus the stabilization of all intermediates necessarily involves several cultures. Figure 2 shows the significance of acetic and propionic acids as intermediate products (10).

We shall implement this scheme in the kinetic model by using the following monenclature.

S = raw material to be converted,

A = acid producing bacteria,

R = intermediate product. It undergoes fast conversion by methane-producing bacteria,

U = intermediate product. It undergoes slow conversion by methane-producing bacteria,

B = methane producing bacteria fermenting R,

C = methane producing bacteria fermenting U,

P = final product.

Figure 3 is a schematic representation of the mixed culture model which is assumed in this study. Although there are a large number of intermediates and microbial species, we shall assume that the system can be adequately represented by two intermediates, R and U, and three microbial species, A, B and C. Figure 4 shows the system of two completely mixed tanks in which the porcess is carried out. Such a system, when it does not include a recycle

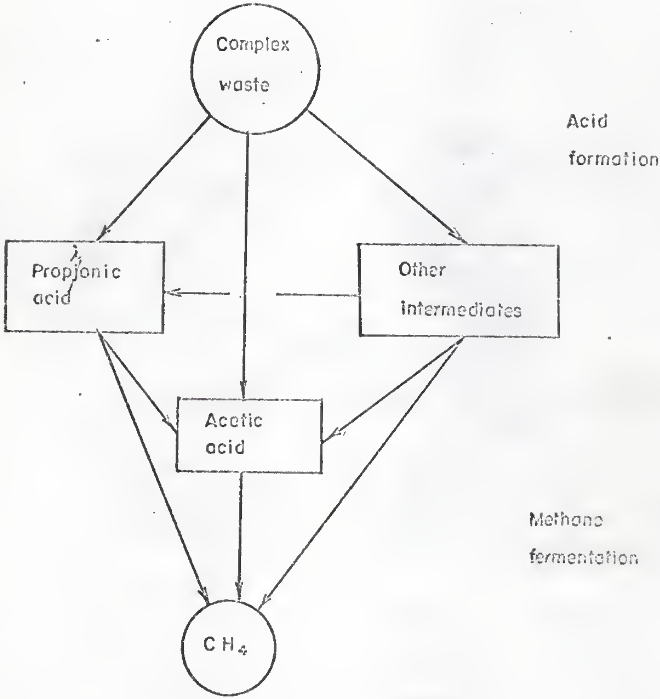


Fig. 2 Pathways in methane fermentation of complex wastes (10).

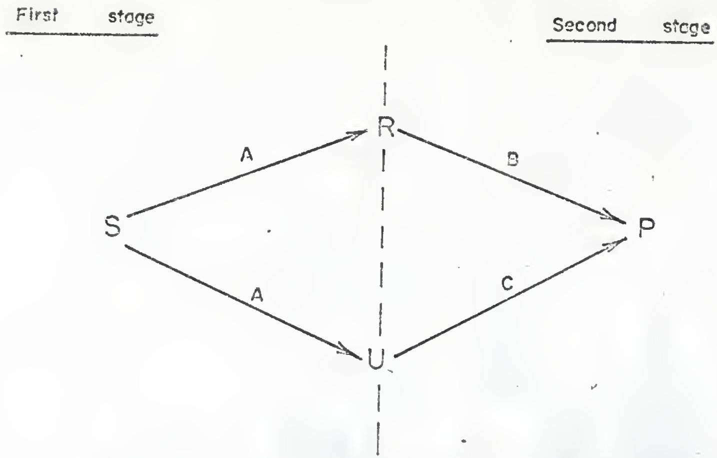


Fig. 3 Mixed culture model used in this study (8).

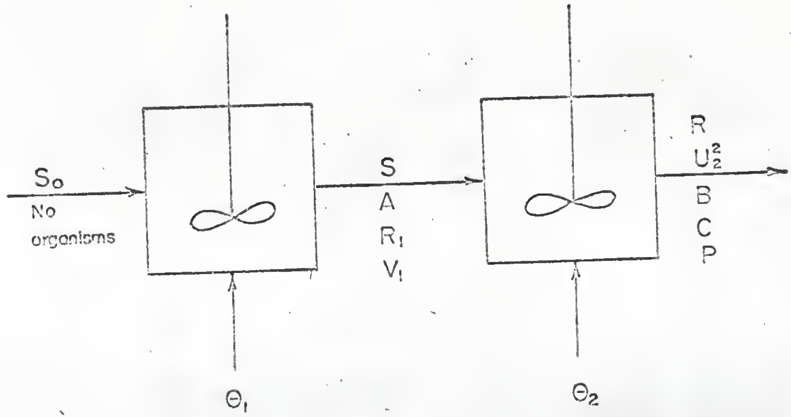


Fig. 4. Conventional two-stage digester system for anaerobic waste water treatment.

stream of organisms, is referred to as a "conventional system" (10). When it includes a recycle stream of organisms, it is a "contact process" (Figure 5).

2. Kinetic model

Several assumptions must be made in developing the kinetic model for this mixed culture system.

1. Environmental conditions are such that acid fermentation occurs only in digestor 1 and methane fermentation only in digester 2.

2. Both digesters are completely mixed.

3. The effect of endogeneous respiration or organism deday can be neglected.

4. Product fermentation is directly related to growth.

5. Isothermal conditions are assumed and thus there is no temperature effect.

6. Monod's function describes the growth rate, i. e.

$$r_x = \frac{kSX}{K_s + X}$$

where

r = rate of production of organism,

k = maximum specific growth rate,

K_s = saturation constant,

S = substrate concentration,

X = organism concentration.

For the sake of clearness, we shall denote the various conversions involved in the kinetic scheme as follows:

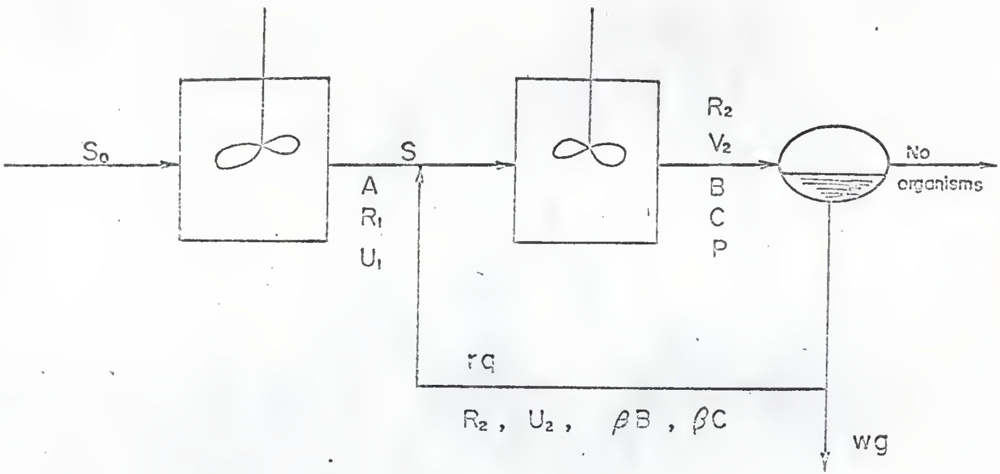


Fig. 5. Anaerobic contact process.

$$\text{(A1)} \quad S \xrightarrow{A} R$$

$$\text{(A2)} \quad S \xrightarrow{A} U$$

$$\text{(B)} \quad R \xrightarrow{B} P$$

$$\text{(C)} \quad U \xrightarrow{C} P$$

Consider conversions (A1) and (A2), where S is metabolized by organism A yielding products R and U and additional cells A. The rates of utilization and creation of the various species involved are directly ralated by the yield factors. The same holds for conversions (B) and (C). For instance, yield factors $Y_{A/S}$ and $Y_{R/S}$ are defined as

$$Y_{A/S} = \frac{\text{rate of formation of A}}{\text{rate of utilization of S}}$$

$$Y_{R/S} = \frac{\text{rate of formation of R by reaction (A1)}}{\text{rate of utilization of S}}$$

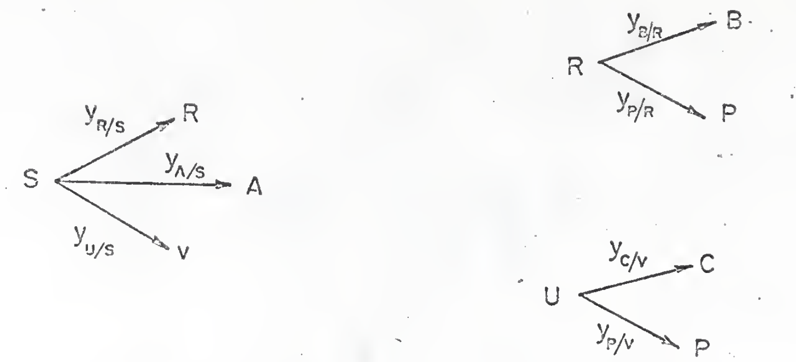
The various yield factors are shown in Figure 6.

In the first stage, substrate S is consumed by organism A, giving organic acids R and U as products. Using Monod's model for growth of A gives

$$r_A = \frac{k_A\ S_1 A}{K_S + S_1} \tag{1}$$

From this expression and the yield factor $Y_{A/S}$, we obtain for the consumption of substrate $(-r_s)$

$$r_s = -\frac{k_A\ S_1 A}{Y_{A/S}(K_S + S_1)} \tag{2}$$



First tank

Second tank

Fig. 6 Yield factors.

Since the rate of production of organic acids R and U is directly related to growth

$$r_{R_1} = - Y_{R/S}\, r_S = \frac{Y_{R/S}}{Y_{A/S}}\, r_A \tag{3}$$

$$r_{U_1} = - Y_{U/S}\, r_S = \frac{Y_{U/S}}{Y_{A/S}}\, r_A \tag{4}$$

In the second stage, intermediate R is consumed by organism B and intermediate U is consumed by organism C with product P (methane) being produced. The kinetic models for growth of organism B and consumption of R are, respectively (the consumption of R is $- r_{R_2}$)

$$r_B = \frac{k_B R_2 B}{K_R + R_2} \tag{5}$$

$$r_{R_2} = - \frac{k_B R_2 B}{Y_{B/R}(K_R + R_2)} \tag{6}$$

Likewise, for organism C and intermediate U, we can write

$$r_C = \frac{k_C U_2 C}{K_U + U_2} \tag{7}$$

$$r_{U_2} = - \frac{k_C U_2 C}{Y_{C/U}(K_U + U_2)} \tag{8}$$

Since product P is produced by the fermentation of both B and C, the expression for product yield is of the form

$$r_P = - Y_{P/R}\, r_{R_2} - Y_{P/U}\, r_{U_2} \tag{9}$$

or in terms of organisms B and C

$$r_P = \frac{Y_{P/R}}{Y_{B/R}} r_B + \frac{Y_{P/U}}{Y_{C/U}} r_C \tag{10}$$

In the next section, these equations will be combined with the material balances at each stage for each species involved in the process. This will yield the performance equations of the system.

3. Performance equations

The material balance equations are derived first for a conventional system (see Figure 4). Then they will be developed for an anaerobic contact process (see Figure 5)

A. Conventional system.

At the first stage, the four species involved are organism A and organics S, R and U. A material balance for organism A yields

$$-A + r_A \theta_1 = 0$$

or

$$A = r_A \theta_1 \tag{11}$$

Substituting r_A from equation (1), and solving for S_1, we have

$$S_1 = \frac{K_S}{\theta_1 k_A - 1} \tag{12}$$

A substrate S material balance gives

$$S_0 - S_1 + r_S \theta_1 = 0$$

or

$$S_0 - S_1 = -r_S \theta_1 \tag{13}$$

Dividing equation (11) by equation (13) gives

$$A = (S_0 - S_1)\left(-\frac{r_A}{r_S}\right)$$

But, by definition $-\frac{r_A}{r_S} = Y_{A/S}$. Therefore we have

$$A = Y_{A/S}(S_0 - S_1) \tag{14}$$

A substrate R material balance for the first stage yields

$$-R_1 + r_{R_1}\theta_1 = 0$$

or

$$R_1 = r_{R_1}\,\theta_1 \tag{15}$$

Dividing equation (15) by equation (13) gives

$$R_1 = (S_0 - S_1)\left(-\frac{r_{R_1}}{r_S}\right)$$

By definition

$$-\frac{r_{R_1}}{r_S} = Y_{R/S}$$

This gives

$$R_1 = Y_{R/S}(S_0 - S_1) \tag{16}$$

In the present kinetic scheme, the processes of formation of R and U are formally identical. Therefore, we can write

$$U_1 = Y_{U/S}(S_0 - S_1) \tag{17}$$

In the second stage, five species are involved, namely B, C, R, U and P. We can write the steady state material balances for each component as follows: For organism B we obtain

$$- B + r_B \theta_2 = 0 \quad (18)$$

or

$$R_2 = \frac{K_R}{k_B \theta_2 - 1} \quad (19)$$

Consider, the consumption of substrate U by organism C. The kinetic relationship governing this growth process is formally the same as for the reaction of organism B on substrate R [Equations (5) and (7)]. Moreover, the material balance for organism C around the second stage has the same form as equation (18). As a result, we can write

$$U_2 = \frac{K_U}{k_C \theta_2 - 1} \quad (20)$$

The material balance at the second stage for intermediate R is

$$R_1 - R_2 + r_{R_2} \theta_2 = 0 \quad (21)$$

or

$$R_1 - R_2 = - r_{R_2} \theta_2 \quad (22)$$

Combining this with equation (18), we get

$$B = \frac{r_B}{r_{R_2}} (R_1 - R_2) \quad (23)$$

Taking account of equations (5) and (6), we have

$$B = Y_{B/R}(R_1 - R_2) \quad (24)$$

Due to the similarity of the reaction of B on R, and of the reaction of C on U, we can write immediately

$$C = Y_{C/U}(U_1 - U_2) \tag{25}$$

The steady state material balance for product P is

$$- P + r_P\theta_2 = 0 \tag{26}$$

Substituting the right hand side of equation (10) for r_P we obtain

$$P = \frac{Y_{P/R}}{Y_{B/R}} r_B\theta_2 + \frac{Y_{P/U}}{Y_{C/U}} r_C\theta_2$$

Taking account of equation (18) and the corresponding relationship $C = r_C\theta_2$ we obtain after substitution

$$P = \frac{Y_{P/R}}{Y_{B/R}} \cdot B + \frac{Y_{P/U}}{Y_{C/U}} \cdot C \quad , \tag{27}$$

Equation (12), (14), (16), and (17) describe the performance of the first stage while equations (19), (20), (24), (25), and (27) describe the behavior in the second stage for a two stage conventional process. The corresponding set of equations for a contact process which includes a recycle stream of organisms will be derived next.

B. System with recycle.

Since the model for growth used in this study assumes that organism A grows only in stage one and organisms B and C grow only in stage two, any attempts to concentrate the organisms by means of recycle must be carried out by feeding the organisms leaving a stage back to that same stage. The methane producing bacteria represented in this study by organisms B and C often have a smaller maximum specific growth rate than the acid producing organisms (organism A in this study). Because of this, recycle of organisms B and C will be considered in this study as shown in Figure 5. Organisms B and C which metabolize the volatile acids in the second stage, are settled in a clarifier at the outlet of this stage (Figure 5). A fraction r_q of the sludge leaving the clarifier is recycled to the second stage. Such a system is referred to as an "anaerobic contact process" (10). It is assumed that there is no endogoueous decay of organisms. All streams after the second stage are supposed to be equally concentrated in organics S, R and U. The recycle stream does not contain product P. The treated effluent does not contain significant quantities of organisms B or C (Figure 5).

Let

q = fraction of the sludge sent to waste disposal section.

β = clarifier efficiency.

r = recycle ratio.

The kinitic scheme given in Section 2 above remains valid for the present system, i. e. the rates of reaction of the various species involved in the process are given by equations (1) through (10). Similarly, for the first stage, there is no modification to equations (12), (14), (16), and (17) needed, because there is no change in performance at this stage.

The performance equations for the second stage are obtained from the steady state material balances for species B, C, R, U, and P.

The amount of organism B entering the second stage is now $(qr)(\beta B)$. Moreover, the flow rate through this stage is $q(1 + r)$. Hence, the material balance for B can be written as

$$qr\beta B + r_B V_2 - q(1 + r)B = 0 \tag{28}$$

where r_B is given by equation (5). Substituting this expression for r_B into equation (28) and dividing by q yields

$$r\beta B + \frac{k_B R_2 B}{K_R + R_2} \cdot \frac{V_2}{q} - (1 + r)B = 0$$

Rearranging this gives

$$\frac{k_B R_2}{K_R + x_{1R}^2} \cdot \frac{V_2}{q} = 1 + (1 - \beta)r \tag{29}$$

By definition $V_{2/q} = \theta_2$ is the hydraulic residence time at the second stage and

$$\xi = 1 + (1 - \beta)r \tag{30}$$

is a dimensionless factor which depends on β and r. Then, equation (~~16~~ 29) can be written as

$$\frac{k_B R_2 \theta_2}{K_R + R_2} = \xi$$

Solving this equation for R_2 gives

$$R_2 = \frac{K_R \xi}{k_B \theta_2 - \xi}$$

Dividing the numerator and denominator of this fraction by yields

$$R_2 = \frac{K_R}{k_B'\theta_2 - 1} \tag{31}$$

where

$$k_B' = k_B/\varsigma \tag{32}$$

Equation (31) has the same form as equation (19), where k_B is replaced by k_B'. Note that equation (28) may be written, after rearranging, as

$$r_B\theta_2 = \varsigma B \tag{33}$$

In the process of metabolization of species U by organisms C, the underlying kinetic scheme is the same as for the reaction of R and B. Therefore, by analogy, we obtain

$$U_2 = \frac{K_U}{k_C'\theta_2 - 1} \tag{34}$$

where

$$k_C' = k_C/\varsigma \tag{35}$$

The amount of R carried by the recycle stream is $(rq)R_2$. The amount of R leaving the second stage is $q(1 + r)R_2$. Then, the steady state material balance of this compound is

$$rqR_2 + qR_1 + r_{R_2}V_2 - q(1 + r)R_2 = 0 \tag{36}$$

Rearranging equation (36), we obtain

$$r_{R_2}\theta_2 = R_2 - R_1 \tag{37}$$

Dividing equation (33) by equation (37) yields

$$\frac{r_B}{r_{R_2}} = \frac{B\,\xi}{R_2 - R_1}$$

From equations (5) and (6)

$$\frac{r_B}{r_{R_2}} = Y_{B/R}$$

Substituting this value into the preceeding equation yields

$$B = \frac{Y_{B/R}}{\xi}(R_1 - R_2)$$

or

$$B = Y'_{B/R}(R_1 - R_2) \tag{38}$$

where

$$Y'_{B/R} = \frac{Y_{B/R}}{\xi} \tag{39}$$

Equation (38) has the same form as equation (23) where $Y_{P/R}$ is replaced by $Y'_{B/R}$.

The steady state material balance for organics U can be obtained by analogy to the case of organics R. Hence we can write immediately

$$C = Y'_{C/U}(U_1 - U_2) \tag{40}$$

where

$$Y'_{C/U} = \frac{Y_{C/U}}{\xi} \tag{41}$$

For product P, the steady state material balance is

$$-P(1+r)q + r_P V_2 = 0$$

or

$$P = \frac{r_P \theta_2}{1+r} \tag{42}$$

Substituting r_P as given by equation (10), we obtain

$$P = \frac{Y_{P/R} r_B \theta_2}{Y_{B/R}(1+r)} + \frac{Y_{P/U} r_C \theta_2}{Y_{C/U}(1+r)} \tag{43}$$

According to equation (33) we have

$$r_B \theta_2 = \xi B$$

By analogy we can write

$$r_C \theta_2 = \xi C$$

Substituting these expressions into equation (43) yields

$$P = \frac{Y_{P/R}}{(1+r)} \frac{\xi B}{Y_{B/R}} + \frac{Y_{P/U}}{(1+r)} \frac{\xi C}{Y_{C/U}} \tag{44}$$

Let

$$Y'_{P/R} = \frac{Y_{P/R}}{1+r}$$

$$Y'_{P/U} = \frac{Y_{P/U}}{1+r} \tag{45}$$

Then, taking account of equations (39), (41), and (45), equation (44) can be written as

$$P = \frac{Y'_{P/R}}{Y'_{B/R}} \cdot B + \frac{Y'_{P/U}}{Y'_{C/U}} \cdot C \tag{46}$$

Performance equations (31), (34), (38), (40) and (46) have the same form as the corresponding equations for the conventional process, i. e. equations (10), (20), (24), (25) and (27) respectively. Therefore, provided the constants k_B, k_C, $Y_{B/R}$, $Y_{C/U}$, $Y_{P/R}$ and $Y_{P/U}$ are transformed according to equations (32), (35), (39), (41) and (45) respectively, the simulation of the process can be carried out using the same computer program as for the conventional process.

An important parameter for a contact process is the solid retention time. According to McCarty (10), the solid retention time (SRT) is defined as

$$SRT = \frac{\text{Suspended solids in the system}}{\text{Suspended solids removed per day}}$$

We shall apply this definition to the organisms B in the second stage. The mass of organisms B in this stage is V_2B. The quantity of B removed per day is $(\ q)(\beta B)$. Then

$$SRT_B = \frac{V_2B}{\omega q \beta B}$$

or

$$SRT_B = \frac{V_2}{q} \cdot \frac{1}{\omega\beta} \tag{47}$$

where SRT_B is the solid retention time of organisms B in the second stage. Furthermore the material balance for organisms B around the clarifyer can be expressed as

$$(1 + r)\, qB = (r + \omega)\, q\beta B$$

which yields, after simplifying and rearranging,

$$\beta\omega = 1 + (1 - \beta)\, r \tag{48}$$

Then, according to equations (30), (47), and (48), SRT_B can be expressed as

$$SRT_B = \frac{\theta^2}{\xi}$$

Note that equation (48) implies

$$1 + (1 - \beta)\, r > 0$$

or

$$r < r_{max}$$

where

$$r_{max} = \frac{1}{\beta - 1}$$

When $r = r_{max}$, equation (48) shows that

$$\beta\omega = 0$$

If $\beta \neq 0$, then $\omega = 0$, i. e. all available organisms B are recycled.

C. Concept of wash-out time.

Since microbial growth is an autocatalytic process, organisms must be present for growth to occur. If the flow rate is too large relative to the reproduction rate the organisms may not be able to reproduce fast enough and wash-out of organisms may result. It is important to determine which residence times will continuously support a growing culture and which ones will result in wash out and no growth. At first we shall consider the first stage. The function which describes the variations of outlet concentration of substrate S is hyperbolic as given by equation (12).

$$S_1 = \frac{K_S}{\theta_1 k_A - 1} \tag{12}$$

There is a mathematical limit for θ_1 for which $S_1 \rightarrow \infty$. This occurs where $\theta_1 \rightarrow 1/k_A$. Obviously, it has no physical significance since $S_1 < S_0$. The lowest residence time θ_{w1} for which equation (12) has a physical significance is where

$$S_1 = S_0$$

This is to say that, when $\theta_1 = \theta_{w1}$, wash-out occurs for organism A and there is no conversion of substrate S. Equations (16), (17), and (14) show that under this condition $R_1 = U_1 = A = 0$. These results are illustrated in Figure 7. When $\theta_1 > \theta_{w1}$. Organism A can grow and S is converted to produce R and U. Equations (12), (14), (16), (17) show that, under this condition, we have

$$S_1 < S_0, \text{ and } \quad \begin{cases} A > 0 \\ R_1 > 0 \\ U_1 > 0 \end{cases}$$

At the inlet of the second stage the concentration of S, A, R, and U are respectively S_1, A, R_1, and U_1. Consider equation (19) which gives R_2, the outlet concentration of R, as a function of residence time θ_2 in the second stage. As in the

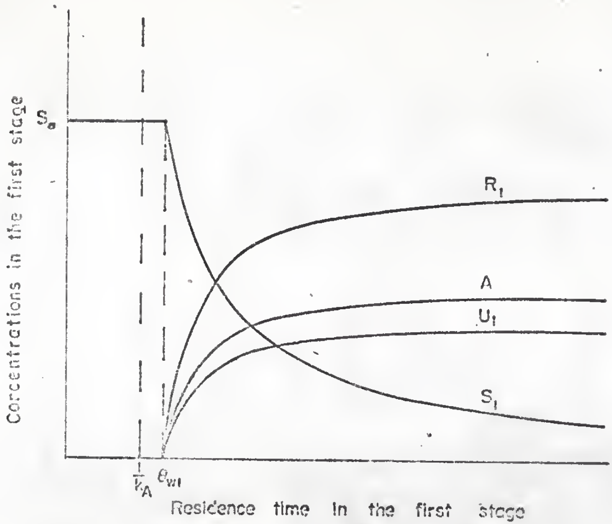


Fig. 7 Wash-out time for the first stage.

previous case the relative size of the values of the maximum specific growth rate k_B and the dilution rate θ_2 will determine whether growth of organism B can occur in the second tank. R is converted only if organism B is present in which case the inlet concentration R_1 exceeds the outlet concentration R_2. Examining equation (19) then shows that there exists a residence time θ_{wz} for which the following equation holds.

$$R_2 - R_1 = 0 \tag{49}$$

At θ_{w2}, equation (23) shows that $B = 0$. When $\theta_2 > \theta_{w2}$, R begins to be converted and B to grow, giving product P.

A similar reasoning applies to U and C. The former is converted and the latter grows only if $\theta_2 > \theta_{w3}$, where θ_{w3} is the solution of equation (20) for θ_2 if

$$U_2 = U_1 \tag{50}$$

At θ_{w3}, equation (25) shows that $C = 0$. When $\theta_2 > \theta_{w3}$, U begins to be converted, and C to grow, yielding product P.

It has been noted (8) that in the second stage, wash-out usually occurs first for the organism which has the smallest maximum specific growth rate. Since $k_C < k_B$, C is the slowest growing organism. Therefore, the following inequality is usually satisfied.

$$\theta_{w2} < \theta_{w3} \tag{51}$$

Thus, the condition which must be satisfied in order for organism A to grow in the first stage is

$$\theta_1 > \theta_{w1} \tag{52}$$

Similarly, the condition for the growth of organisms B and C in the second stage is

$$\theta_2 > \theta_{w3} \tag{53}$$

The inequalities given by equations (52) and (53) will be referred to as "conditions of feasibility".

4. Economic model.

We shall consider a cost of treatment consisting of two terms. The first term is the total hydraulic residence time $\theta_1 + \theta_2$ of the feed stream q in the system. This term represents approximately the cost of the digesters in terms of volume. Therefore, it also represents roughly the fixed costs of treatment for a given plant and a given flow rate. In addition, the degree of removal of organics from the feed stream has an important economic significance. In fact, the stream leaving the clarifier can either be discharged into a receiving stream or treated further in order to achieve a better stabilization of its organic content. In both cases, we may incur a penalization which is a function of the degree of treatment. In this work, the penalization term takes the form $z_S S_1 + z_R R_2 + z_U U_2$ penalization where z_S, z_R, and z_U are constants. This term must also be expressed in terms of residence time. Thus, the dimension of the constants z_S, z_R, and z_U is time/concentration.

III. ANALYSIS OF SYSTEM

In this section, we shall determine the wash-out times, θ_{w1}, θ_{w2}, θ_{w3}, of the system using the concept of wash-out stated in Section II.3. Then, we shall prove that the wash-out steady state is a solution for the steady state problem provided that the feed stream is free of organisms.

1. <u>Determination of wash-out times.</u>

Organism A:

By definition of θ_{w1}, we have

$$S_1(\theta_{w1}) = S_0$$

Because of equation (12), this gives

$$\frac{K_S}{\theta_{w1}\, k_A - 1} = S_0$$

and

$$\theta_{w1} = \frac{1}{k_A}\left(1 + \frac{K_S}{S_0}\right) \tag{54}$$

K_S and S_0 are positive. Thus, equation (54) implies

$$\theta_{w1} > \frac{1}{k_A} \tag{55}$$

Moreover, when $S_1 = S_0$, equation (14) shows that $A = 0$. When wash-out occurs in the first stage, the concentration of organism A is zero.

Organism B:

The corresponding wash-out time, say θ_{w2}, occurs when

$$R_2(\theta_{w2}) = R_1 \tag{56}$$

Substituting from equation (19), we have

$$\frac{K_R}{k_B\,\theta_{w2} - 1} = R_1$$

Then

$$\theta_{w2} = \frac{1}{k_B}\left(1 + \frac{K_R}{R_1}\right) \tag{57}$$

Again, we notice that substituting equation (56) into equation (24) leads to B = 0.

Organism C:

θ_{w3} corresponds to the condition that

$$U_2(\theta_{w3}) = U_1 \tag{58}$$

Substituting from equation (20) we have

$$\frac{K_U}{k_C\,\theta_{w3} - 1} = U_1$$

Solving for θ_{w3} yields

$$\theta_{w3} = \frac{1}{k_C}\left(1 + \frac{K_U}{U_1}\right) \tag{59}$$

This equation implies that

$$\theta_{w3} > \frac{1}{k_C} \tag{60}$$

Equation (54) shows that θ_{w1} does not depend on the residence time of any of the stages. However, the expressions for θ_{w2} and θ_{w3} contain the terms R_1 and U_1 respectively, which are dependent on the residence time of the first stage. As a result, the wash-out times of organisms B and C depend on the residence time in the first tank. Figure 8 illustrates the concept of wash-out time of organism A in the first stage. The dimensionless concentrations S_1/S_0, A/S_0, E_1/S_0, and U_1/S_0 as obtained from equations (12), (14), (16), and (17) respectively are plotted versus the residence time θ_1 ranging from 0 to 2 days. When $\theta_1 < \theta_{w1}$, $S_1/S_0 = 1$ and $A/S_0 = 0$, no conversion takes place and wash-out of organism A occurs. When $\theta_1 > \theta_{w1}$, the concentration of substrate S falls, indicating that S is converted, while the concentration of organism A rises due to its growth.

2. Steady state wash-out time.

Let us consider the first stage. If we assume an initial concentration A_0 of organisms in the feed stream, the material balance for organism A can be written as

$$A_0 - A = - r_A \theta_1 \tag{61}$$

For substrate S, it is

$$S_0 - S_1 = -r_S \theta_1 \tag{7}$$

Dividing equation (61) by equation (7) and noting that $-r_A/r_S = Y_{A/S}$, we obtain

$$A_0 - A = - Y_{A/S}(S_0 - S_1) \tag{62}$$

which can be rearranged to give

$$A = A_0 + Y_{A/S}(S_0 - S_1)$$

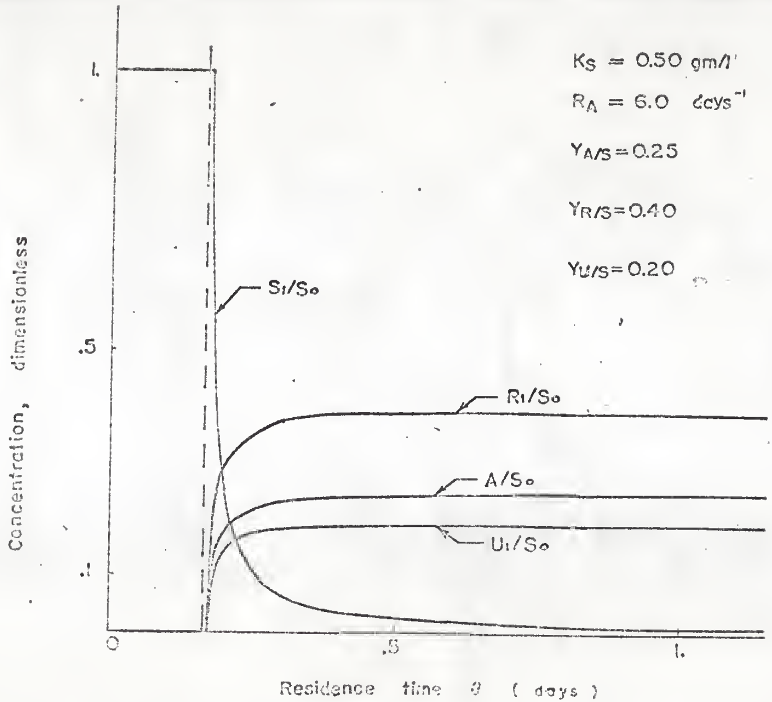


Fig. 8 Dimensionless concentrations of S, R, U, and A in the first stage.

Substituting this expression into equation (1) giving r_A yields

$$r_A = \frac{k_A S_1}{K_S + S_1} [A_0 + Y_{A/s}(S_0 - S_1)] \tag{63}$$

Substituting equations (62) and (63) into equation (61) yields

$$- Y_{A/S}(S_0 - S_1) = - \frac{k_A\ \theta_1\ S_1}{K_S + S_1} [A_0 + Y_{A/S}(S_0 - S_1)] \tag{64}$$

By introducing the condition $A_0 = 0$, equation (64) can be written as

$$(S_0 - S_1)(1 - \frac{k_A\ \theta_1\ S_1}{K_S + S_1}) = 0 \tag{65}$$

This is an equation of second order, which gives the steady state concentration S_1. Obviously, one of the roots is $S_1 = S_0$. This is precisely the condition for wash-out of organism A from the first stage. Another root is given by

$$1 - \frac{k_A\ \theta_1\ S_1}{K_S + S_1} = 0$$

Solving for S_1 yields

$$S_1 = \frac{K_S}{\theta_1\ k_A - 1} \tag{12}$$

which is identical to equation (12). Thus this approach shows that, in addition to the steady state described by the performance equations given in Section II.3., there is a second solution which can be referred to as "wash-out steady state" for the first stage. By analogy the same conclusions can be reached for the second stage.

The analysis given above yields an important conclusion as to the operation of the system. Indeed, let us assume that wash-out of organism A occured in the first stage due to flooding. Then, for this stage, the stable steady state solution is given by the first root of equation (65), i.e. $S_1 = S_0$. This implies that the feed stream flow through the first stage without undergoing any biochemical conversion. However, if a residence time θ_1 is established such that $\theta_1 > \theta_{w1}$ and if some organism A is introduced into the first stage, this organism can grow utilizing substrate S. After a transient period, the system reaches a stable steady state described by the second root of equation (65) which yields equation (12). In this steady state, continuous organic utilization occurs, which is the condition for the system to operate efficiently.

IV. OPTIMIZATION

In this Section, we shall determine the optimal policy for a two-stage continuous anaerobic digester system using two different approaches. In the first approach, differential calculus yields an analytical expression for the optimal policy. In the second approach, the analysis of the problem is carried out from the point of view of an empirical search technique, namely the Simplex technique which is discussed in Appendix IV.

1. Formulation of the problem

According to the economic model described in Section II.4, the objective function to be minimized consists of two parts. The first part expresses the equipment cost $(\theta_1 + \theta_2)$. The second part is the penalization cost $z_S S_1 + z_R R_2 + z_U U_2$ for discharging the organics remaining in the effluent stream. Thus the objective function J can be expressed as

$$J = \theta_1 + \theta_2 + z_S S_1 + z_R R_2 + z_U U_2 \tag{66}$$

Substituting equations (12), (19), and equation (20) into the above equation gives

$$J = \theta_1 + \theta_2 + \frac{z_S K_S}{\theta_1 k_A - 1} + \frac{z_R K_R}{k_B \theta_2 - 1} + \frac{z_U K_U}{k_C \theta_2 - 1} \tag{67}$$

Note that if $\theta_{w2} \leq \theta_2 < \theta_{w3}$, the concentration of U in the treated effluent is U_1. Then the objective function would be

$$J' = \theta_1 + \theta_2 + \frac{z_S K_S}{\theta_1 k_A - 1} + \frac{z_R K_R}{k_B \theta_2 - 1} + z_U U_1$$

The decision variables are chosen to be the two residence times θ_1 and θ_2. Since there is no equality constraint, the optimization problem is two-dimensional. Equation (67) shows that the optimization problem is a non-linear one with the decision variables θ_1 and θ_2 subject to the conditions of feasibility.

$$\theta_1 > \theta_{w1} \tag{52}$$

$$\theta_2 > \theta_{w3} \tag{53}$$

2. <u>Numerical data</u>.

The optimization will be performed with the following values of physical and economical parameters:

$S_0 = 10.0$ gm/l
$k_A = 6.0$ day^{-1}
$K_S = 0.50$ gm/l
$Y_{A/S} = 0.25$
$Y_{R/S} = 0.40$
$Y_{U/S} = 0.20$
$k_B = 0.50$ day^{-1}
$K_R = 1.00$ gm/l
$Y_{B/R} = 0.10$
$Y_{P/R} = 0.75$
$k_C = 0.25$ day^{-1}
$K_U = 1.50$ gm/l
$Y_{C/U} = 0.10$
$Y_{P/U} = 0.75$
$z_S = 1.00$
$z_R = 1.50$
$z_U = 1.50$

The choice of these values for z_S, z_R, and z_U is compatible with the two conditions of feasibility as will be shown in Section IV. 3 below.

3. Analysis by differential calculus.

Let (Σ) be the surface described by equation (67). First, we have to find the stationary points on surface (Σ). The coordinates of such points satisfy the necessary conditions

$$\frac{\partial J}{\partial \theta_1} = 0 \tag{68}$$

and

$$\frac{\partial J}{\partial \theta_2} = 0 \tag{69}$$

From equation (66) we have

$$\frac{\partial J}{\partial \theta_1} = 1 + z_S \frac{dS_1}{d\theta_1} + z_R \frac{dR_2}{d\theta_1} + z_U \frac{dU_2}{d\theta_1}$$

R_2 and U_2 do not depend on θ_1. Then substituting $dS_1/d\theta_1$ yields

$$1 - \frac{z_S\ K_S\ k_a}{(k_A\ \theta^1 - 1)^2} = 0 \tag{70}$$

Solving for θ_1 yields

$$\theta_1 = \frac{1}{k_A}[1 \pm \sqrt{z_S\ K_S\ k_A}] \tag{71}$$

In order for θ_1 to have a physical significance, it has to satisfy

$$\theta_1 > \theta_{w1} > \frac{1}{k_A}$$

Therefore, the expression for θ_1 is necessarily

$$\theta_{1L} = \frac{1}{k_A}[1 + \sqrt{z_S\ K_S\ k_A}\ ] \tag{72}$$

Let us now consider equation (69). From equation (66)

$$\frac{\partial J}{\partial \theta_2} = 1 + z_R \frac{dR_2}{d\theta_2} + z_U \frac{dU_2}{d\theta_2}$$

Substituting into this equation the derivatives $\frac{dR_2}{d\theta_2}$ and $\frac{dU_2}{d\theta_2}$ computed from equations (19) and (20) yields

$$\frac{\partial J}{\partial \theta_2} = 1 - \frac{z_R\ K_R\ k_B}{(k_B\ \theta_2 - 1)^2} - \frac{z_U\ K_U\ k_C}{(k_C\ \theta_2 - 1)^2} = 0$$

or

$$\frac{z_R\ K_R\ k_B}{(k_B\ \theta_2 - 1)^2} + \frac{z_U\ K_U\ k_C}{(k_C\ \theta_2 - 1)^2} - 1 = 0 \tag{73}$$

Let

$$\varphi(\theta_2) = \frac{z_R\ K_R\ k_B}{(k_B\ \theta_2 - 1)^2} + \frac{z_U\ K_U\ k_C}{(k_C\ \theta_2 - 1)^2} - 1 \tag{74}$$

Then, equation (74) becomes

$$\varphi(\theta_2) = 0. \tag{75}$$

Equation (73) can also be written as

$$z_R\ K_R\ k_B(k_C\ \theta_2 - 1)^2 + z_U\ K_U\ k_C(k_B\ \theta_2 - 1)$$

$$- (k_B\ \theta_2 - 1)^2(k_C\ \theta_2 - 1)^2 = 0$$

This equation is of 4th order and, therefore, equation (73) has four roots.

In order for θ_2 to have a physical significance, it has to satisfy

$$\theta_2 > \theta_{w3} > \frac{1}{k_C}$$

It can be shown (see Appendix II) that the largest root of equation (73), say θ_{2L}, always satisfies this condition. It remains to prove that the point defined by the coordinates θ_{1L} and θ_{2L} is a minimum on response surface (Σ), i.e. that the Hessian matrix of the objective function J is positive definite at this point (see Appendix III).

Equations (72) and (75) allow us to express the inequality constraints (52) and (53) in terms of the physical and economical parameters of the system.

The first inequality constraint is

$$\theta_{1L} > \theta_{w1}$$

Substituting equations (54) and (72) in this equation leads to the relationship

$$\frac{1}{k_A}\left[1 + \sqrt{z_S\, K_S\, k_A}\,\right] > \frac{1}{k_A}\left[1 + \frac{K_S}{S_0}\right]$$

which must be satisfied to have growth in the first tank.

Simplification of the above relation yields

$$\sqrt{z_S\, K_S\, k_A} > \frac{K_S}{S_0}$$

Raising this to the second power and rearranging gives

$$z_S\, k_A\, (S_0)^2 - K_S > 0 \qquad (76)$$

Values of all the parameters appearing in this inequality are positive. It follows from inequality given by equation (76) that

$$z_S > \frac{K_S}{k_A\, (S_0)^2}$$

For a given initial substrate concentration, there is a lower limit for penalization z_S in order for the first stage to operate above the wash-out residence time and under optimal conditions $z_S = 1.0$ satisfies the inequality of equation (76).

The second inequality constraint is

$$\theta_{2L} > \theta_{w3} \tag{77}$$

where θ_{2L} is the largest root of $\varphi(\theta_2) = 0$ and θ_{w3} is given by equation (59). We know that θ_{w3} and θ_{2L} are both larger than $1/k_C$, and that $\varphi(\theta_2)$ monotonously decreases when $\theta_2 > 1/k_C$. Therefore, the inequality given by equation (77) yields

$$\varphi(\theta_{w3}) > \varphi(\theta_{2L})$$

But, by definition,

$$\varphi(\theta_{2L}) = 0$$

Hence, the second condition for feasibility is

$$\varphi(\theta_{w3}) > 0$$

Substituting the expression for φ from equation (74) yields

$$\frac{z_R\ K_R\ k_B}{(k_B\ \theta_{w3} - 1)^2} + \frac{z_U\ K_U\ k_C}{(k_C\ \theta_{w3} - 1)^2} - 1 > 0 \tag{78}$$

This inequality is linear in z_R and z_U. In addition, θ_{w3} depends on θ_1. It can thus be concluded that for given operating conditions at the first stage, there are lower limits for penalization coefficients z_R and z_U. $z_R = z_U = 1.50$ satisfies the inequality given by equation (78).

Finally, the coordinates θ_{1L} and θ_{2L} of point A minimize the objective function J given by equation (67) and satisfy the inequality constraints given by equations (52) and (53). Thus,

$$\theta_{1OPT} = \theta_{1L}$$

$$\theta_{2OPT} = \theta_{2L}$$

Point A corresponds to the optimal policy on response surface (Σ). In addition to point A, the surface (Σ) has three other stationary points, namely, B, C, and D (see Appendix III). B and D are saddle points, C is a maximum point.

4. <u>Analysis by empirical search</u>.

As stated previously the objective function J is to be minimized under the two inequality constraints $\theta_1 > \theta_{w1}$ and $\theta_2 > \theta_{w3}$, where θ_1 and θ_2 are the two decision variables.

In the differential calculus approach, this constrained optimization problem is solved in two steps. In the first one, we determine the stationary points of the response surface (Σ). In the second one, we check a posteriori that the stationary point of interest (point A) satisfies the inequality constraints given above.

The empirical search technique, Simplex, is particularly suitable to treat at once such a constrained optimization problem (see Appendix IV).

By means of these two techniques, it is found that the optimal residence times for the system under consideration are

$\theta_1 = 0.455$ days and $\theta_2 = 7.183$ days. Figure 9 shows a plot of the dimensionless concentrations R_2/S_0, U_2/S_0, B/S_0, C/S_0 and P/S_0 in stage two for the optimal policy for stage one. Figure 10 shows the plot of the same dimensionless concentration for a contact system where $r = 0.25$ and $\beta = 4.0$. These figures illustrate the increased stability of the contact process. Indeed, the wash-out times θ_{w2} and θ_{w3} for the contact process are 0.629 days and 1.772 days as compared to 2.515 days and 7.087 days for the conventional system. Comparing Figures 9 and 10 shows also a strong increase in organism concentrations B and C together with a more efficient reduction of the organics in the case of the contact process.

5. <u>Contours</u>.

When J is given a fixed value J_c equation (67) represents the corresponding contour. Let us write equation (67) in the form

$$J_c = A + \theta_1 + \frac{z_S\ K_S}{k_A\ \theta_1 - 1} \tag{79}$$

where

$$A = \theta_2 + \frac{z_R\ K_R}{k_B\ \theta_2 - 1} + \frac{z_U\ K_U}{k_C\ \theta_2 - 1} \tag{80}$$

Rearranging equation (79) yields

$$k_A(\theta_1)^2 + [(A - J_c)\ k_A - 1]\theta_1 + z_S\ K_S + J_c - A = 0 \tag{81}$$

For the purpose of generation of the contours, let y be the current value of θ_2, and x_1 and x_2 the current values of the

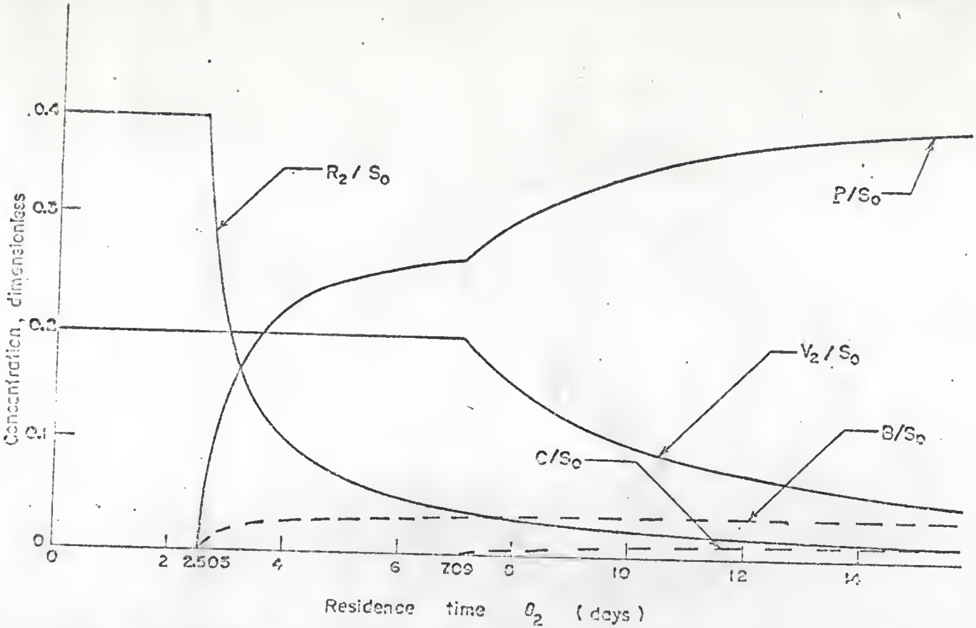


Fig. 9 Dimensionless concentration curves for the second stage for the optimal policy (conventional process).

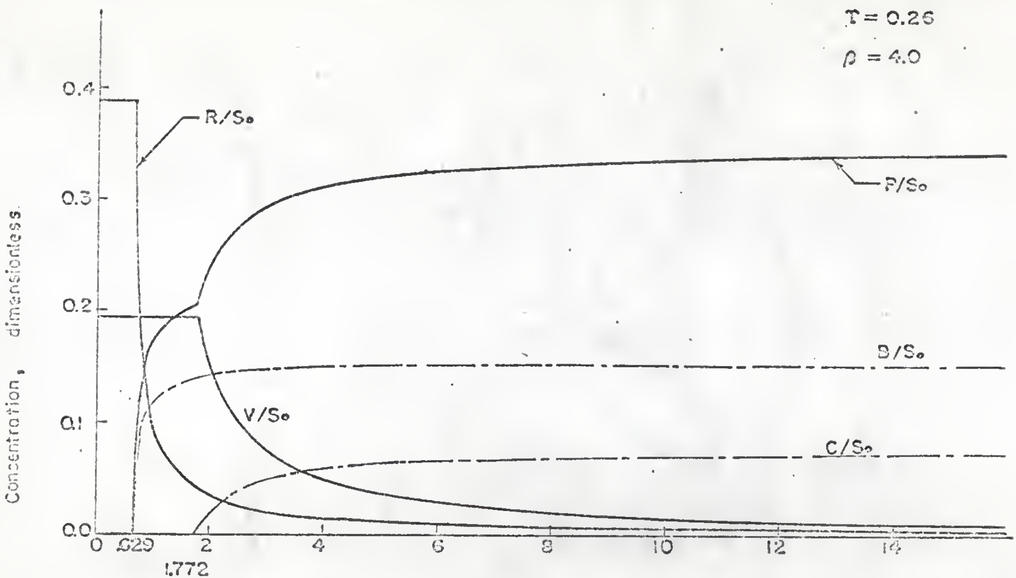


Fig. 10. Dimensionless concentration curves for the second stage for the optimal policy (contact process).

two roots of equation (81). Thus the procedure to get the contour corresponding to J_c is as follows:

Fix y (or θ_2).

Compute A by equation (80).

Substitute A and solve equation (81) for x_1 and x_2.

The two points (x_1, y) and (x_2, y) lie on the contour where the objective function has the value J_c. By allowing y to vary the whole contour is generated. Thus the question arises: what is the permissible range for y? The discriminant of quadratic equation (81) is

$$= [(A - J_c)k_A - 1]^2 - 4k_A(z_S\, K_S + J_c - A)$$

For equation (81) to have two real roots,   has to be positive. This restricts the range of variation of A and θ_2 in case of a maximum or minimum for response surface (Σ).

The contours of response surface (Σ) around the stationary points A, B, C and D are shown on Figures 11, 12, 13, and 14.

On Figure 13, the contours generated by this procedure have no physical significance when $\theta_{w2} < \theta_2 \leq \theta_{w3}$. This part of the contours are represented by the dashed lines. In deed, when $\theta_{w2} < \theta_2 \leq \theta_3$, wash-out occurs for organism C. Thus, the objective function is given by the following equation (see Section IV.)

$$J' = \theta_1 + \theta_2 + \frac{z_S\, K_S}{k_A\, \theta_1 - 1} + \frac{z_R\, K_R}{k_B\, \theta_2 - 1} + z_U\, U_1 \qquad (82)$$

where U_1 is given by

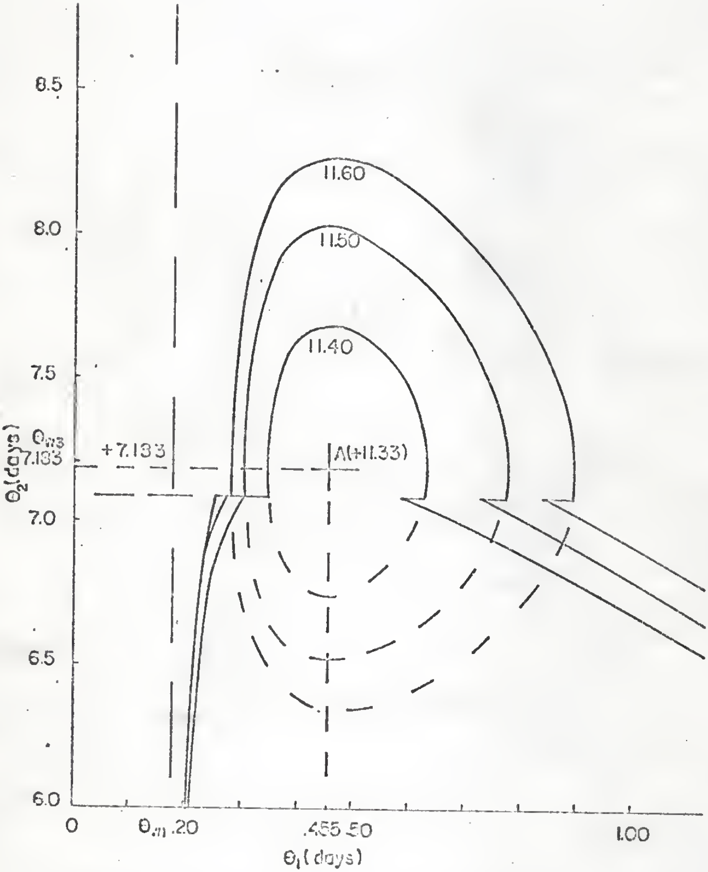


Fig. 11 Contours of the response surface around optimal point A.

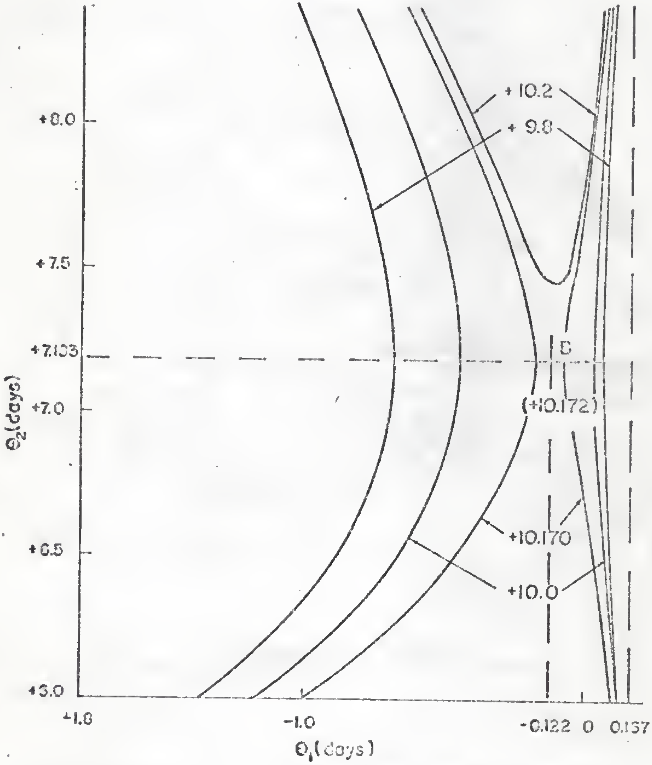


Fig. 12 Contours of the response surface around saddle point B.

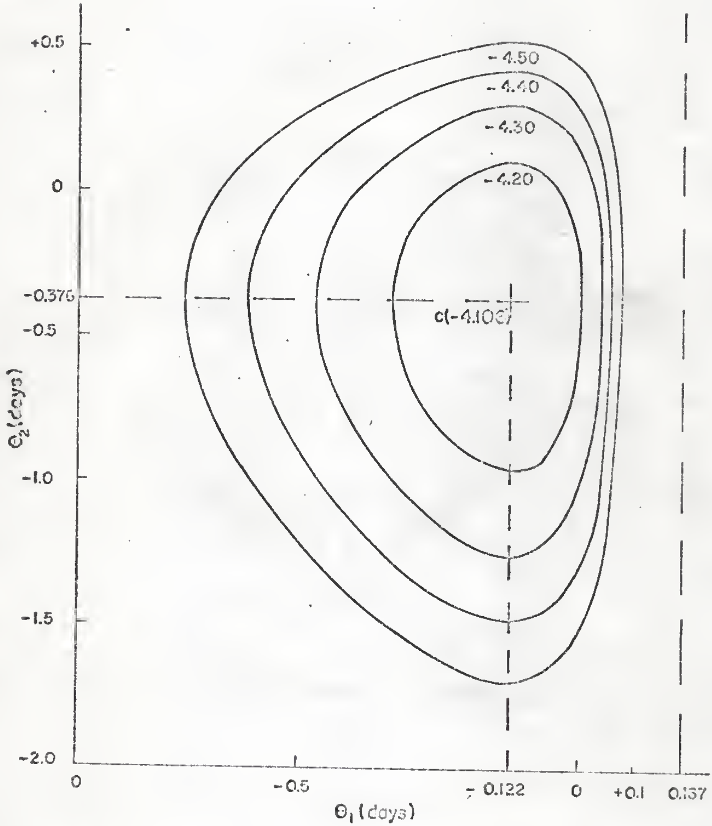


Fig. 13 Contours of the response surface around minimun point C.

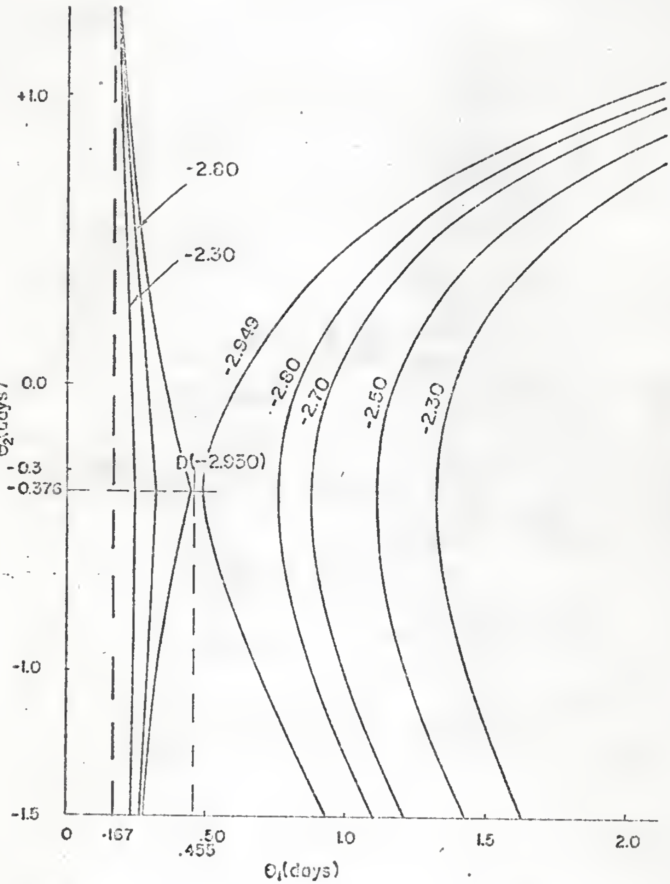


Fig. 14 Contours of the response surface around saddle point D.

$$U_1 = Y_{U/S}\,(S_0 - S_1) \tag{17}$$

and S_1 is given by

$$S_1 = \frac{K_S}{k_A\,\theta_1 - 1} \tag{12}$$

Equations (12) and (17) yield

$$U_1 = Y_{U/S}\,(S_0 - \frac{K_S}{k_A\,\theta_1 - 1})$$

Substituting this expression of U_1 into equation (82) gives

$$J' = \theta_1 + \theta_2 + \frac{z_S\,K_S}{k_A\,\theta_1 - 1} + \frac{z_R\,K_R}{k_B\,\theta_2 - 1}$$

$$+ z_U\,Y_{U/S}(S_0 - \frac{K_S}{k_A\,\theta_1 - 1}) \tag{83}$$

When J' is given a fixed value J'_c, equation (83) represents the corresponding contour. Let us write equation (83) in the form

$$J'_c = A' + \theta_1 + z_S\,K_S - \frac{z_U\,Y_{U/S}\,K_S}{k_A\,\theta_1 - 1} \tag{84}$$

where

$$A' = \theta_2 + \frac{z_R\,K_R}{k_B\,\theta_2 - 1} + z_U\,Y_{U/S}\,S_0 \tag{85}$$

Rearranging equation (84) yields

$$k_A(\theta_1)^2 + [(A' - J'_c)k_A - 1]\theta_1 + z_S\,K_S - z_U\,Y_{U/S}\,K_S$$

$$+ (J'_c - A') = 0 \tag{86}$$

The contours can then be generated using the procedure previously described. They are shown on Figure 13 by the continuous lines where $\theta_2 \leq \theta_{w3}$. The contours of the physical response surface are discontinuous for $\theta_2 = \theta_{w3}$. Indeed, when this equality holds, the expression of the objective function changes. This explains the points of discontinuity on Figure 13.

V. RESULTS AND DISCUSSION

The numerical results of this work have been obtained using the program MICU20 (see Appendix V). The main design variables for the conventional process and a contact process are given below.

For the conventional process, the optimal policy is θ_1 = 0.455 days and θ_2 = 7.183 days. The corresponding concentrations are

- At the first stage:

S_1 = 0.289 gm/l

A = 2.428 gm/l

R_1 = 3.885 gm/l

U_1 = 1.942 gm/l

- At the second stage:

R_2 = 0.386

U_2 = 1.885

B = 0.350 gm/l

C = 0.006 gm/l

P = 2.667 gm/l

The wash-out times are

$\theta_{w1} = 0.175$ days

$\theta_{w2} = 2.515$ days

$\theta_{w3} = 7.089$ days

For the contact process, the results are computed for $r = 0.25$ and $\beta = 4.0$. The optimal policy is $\theta_1 = 0.455$ days and $\theta_2 = 2.64$ days. The corresponding concentrations are

- At the first stage

$S_1 = 0.289$ gm/l

$A = 2.428$ gm/l

$R_1 = 3.885$ gm/l

$U_1 = 1.942$ gm/l

- At the second stage

$R_2 = 0.234$ gm/l

$U_2 = 0.914$ gm/l

$B = 1.460$ gm/l

$C = 0.411$ gm/l

$P = 2.807$ gm/l

The wash-out times are

$\theta_{w1} = 0.175$ days

$\theta_{w2} = 0.629$ days

$\theta_{w3} = 1.772$ days

The solid retention time in the second stage is

$SRT_E = 10.56$ days

A parametric study has been carried out with r as parameter,

β being given a constant value of 4.0. The successive values of r are 0., 0.05, 0.10, 0.15, 0.20, 0.25 and 0.333, respectively. Figure 15, which is a plot of the optimal cost of treatment versus the recycle ratio r. Shows that the cost is significantly reduced by using recycle. Similarly, in Figure 16, a plot of percent of reduction of organics versus the recycle ratio r shows that recycle increases the degree of treatment obtained in an optimum system. Figure 17 which is a plot of total gas production versus r, illustrates the increased gas production obtained by means of recycle. Finally, Figure 18 gives a plot of the wash-out liquid retention time θ_{w3} as a function of the recycle ratio.

As compared to the conventional anaerobic process, the results obtained in this work show that the anaerobic contact process has several advantages under the optimal condition. For a recycle ratio of 0.25 and a clarifier efficiency of 4.0, the cost reduction is (11.333 - 5.106)/11.333 = 54.9%. In the conventional process the concentration of organics in the effluent stream is 0.289 + 0.386 + 1.885 = 2.56 gm/l. The reduction in organics concentration is then (10. - 2.56)/10 = 74.4%. In the contact process the concentration of organics in the outlet stream is 0.289 + 0.234 + 0.914 = 1.437 gm/l which yields a reduction in organics of (10. - 1.437)/10. = 85.6%. The amount of gaseous products is, for the contact process, (1. + .25) x 2.807 = 3.51 gm/l. Thus, there is an improvement in production of gaseous products which can be used to meet the energy requirements of the process. This improvement is (3.51 - 2.667)/ 2.667 = 31.6%. Finally, the wash-out time θ_{w3} decreases from

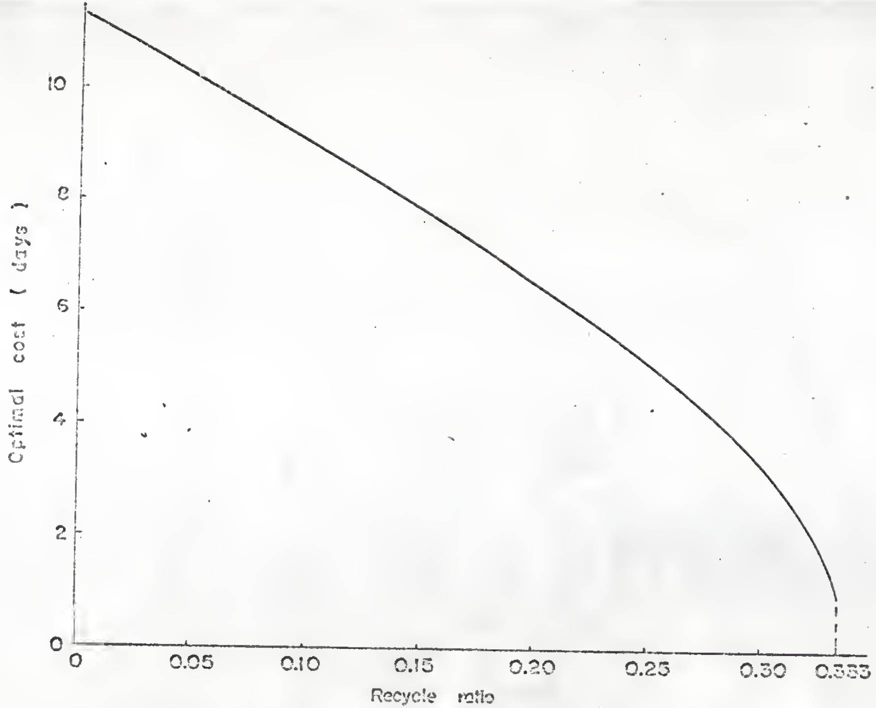


Fig. 15 Plot of optimal cost of treatment vs recycle ratio.

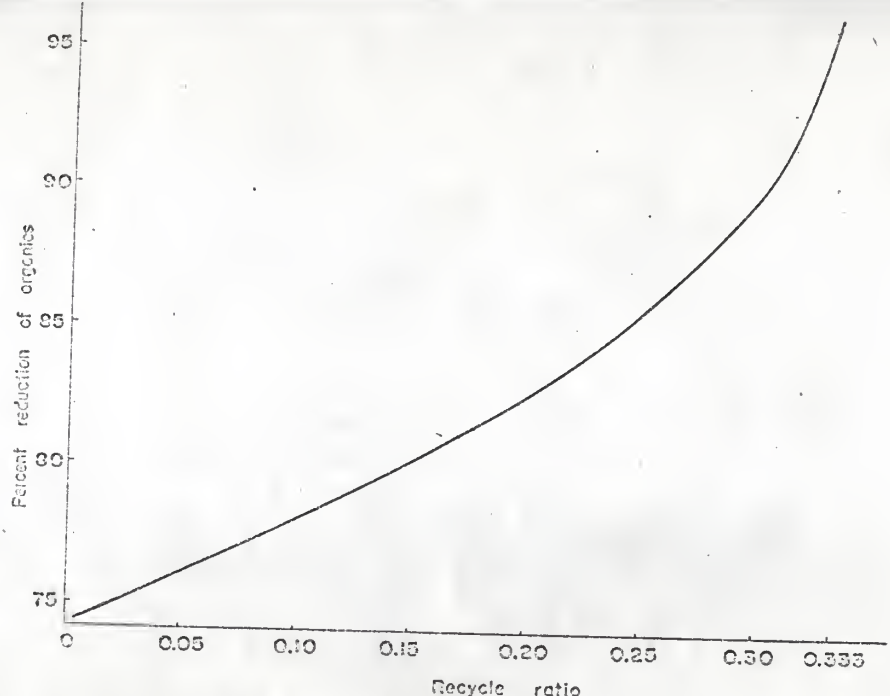


Fig.16 Plot of percent reduction of organics vs recycle ratio.

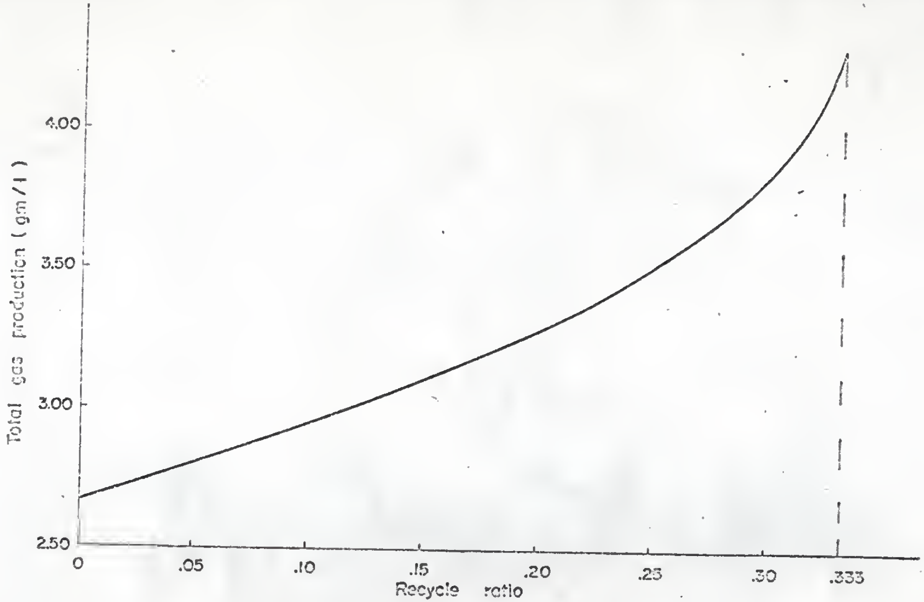


Fig. 17 Plot of total gas production vs recycle ratio for optimal policy.

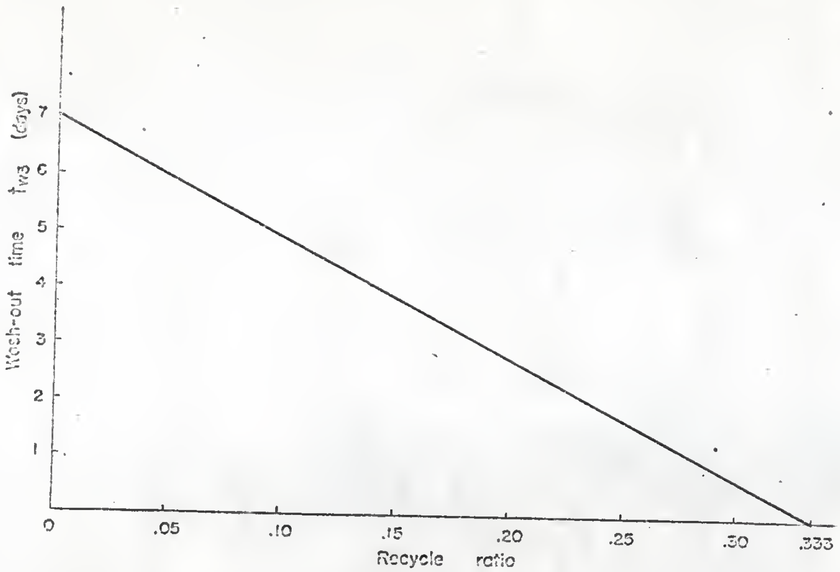


Fig.18 Plot of liquid retention wash out time t_{w3} vs recycle ratio for optimal policy.

7.089 days for a conventional system to 1.772 days for the contact process.

Figures 15 to 18 show that these improvements in the performance of the system take place over the whole permissible range of the recycle ratio. However, the assumption of a constant value for the clarifier efficiency β may not be true when r takes on high values. At these recycle rates, almost all the organisms contained in the stream leaving the second stage have to be separated. Indeed, the major problem arising from the use of the anaerobic contact process to date is related to an inability to separate efficiently the bacterial solids from the effluent stream for recycle back to the second stage (14). High efficiency is necessary to maintain the required long sludge retention time while operating at short hydraulic detention times (14). In the successful full-scale treatment of meat-packing wastes (15), a vacuum degasifier has been used between the digester and final settling tank to remove gases which tend to float the solids rather than allowing them to settle in the settling tank.* This scheme or some other solids separation device may be needed to implement the anaerobic contact process.

Moreover, high values for the recycle ratio imply long solid retention times. This yields organism decay, which is assumed to be negligible in this work. Hence, the curves given

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* A flotation process making use of the large quantities of dissolved gases to float and concentrate the solids for return to the digester also appears feasible (10).

on Figures 15 to 18 are not significant for high values of r. However, they show a realistic trend when the value of r is consistent with the assumptions of constant clarifier efficiency and constant maximum specific growth rate.

VI. CONCLUSIONS

A mathematical formulation of the kinetic model reported by several authors (7, 9, 10) for the anaerobic digestion process allowed us to analyze the two-stage systems under consideration in this work. It has then been shown that the wash-out times are important design parameters. In addition, the process has been optimized by considering an objective function of economic type. Under the assumptions which have been made, the optimization problem has one and only one minimum solution.

As reported by Pfeffer (13), this work shows that the contact process has several advantages over the conventional process. They are more efficient organic content reduction, increased total gas production and greater stability.

This work is a theoretical one. Hence, additional experimental work is required to verify the assumptions which have been made. However, since industrial biological waste treatments involve mixed cultures metabolizing mixed substrates, this study constitutes a contribution to improve our knowledge and control of these processes.

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NOMENCLATURE

q	Flow rate.
S_0	Concentration of organics in the feed stream.
S_1	Concentration of primary substrate in first (and in second) stage.
R_1, U_1	Concentration of volatile acids R and U in first stage.
R_2, U_2	Concentration of volatile acids R and U in the second stage.
P	Concentration of final product in the second stage.
A	Concentration of organism A in the first stage.
B, C	Concentration of organisms B and C in the second stage.
k_A, k_B, k_C	Maximum specific growth rate for organisms A, B, C, respectively.
K_S, K_R, K_U	Saturation constants for S, R, U, respectively.
θ_n	Residence time at stage n.
$\theta_{n\ opt}$	Optimal residence time of stage n.
θ_{w1}	Wash-out retention time for organism A.
θ_{w2}	Wash-out retention time for organism B.
θ_{w3}	Wash-out retention time for organism C.
$Y_{A/S}$	Yield constant for formation of organism A in terms of utilization of substrate S.
$Y_{R/S}$	Yield constant for formation of R from S.
$Y_{U/S}$	Yield constant for formation of U from S.
$Y_{B/R}$	Yield constant for formation of organism B from utilization of intermediate R.
$Y_{C/U}$	Yield constant for formation of organism C from utilization of intermediate U.
$Y_{P/R}$	Yield constant for formation of product P from intermediate R.
$Y_{P/U}$	Yield constant for formation of product P from

	intermediate U.
r	Recycle ratio for the second stage.
β	Clarifyer efficiency.
k'_B, k'_C	Transformed constants for k_B and k_C.
$Y'_{B/R}$	Transformed yield factor for $Y_{B/R}$.
$Y'_{P/R}$	Transformed yield factor for $Y_{P/R}$.
$Y'_{C/U}$	Transformed yield factor for $Y_{C/U}$.
$Y'_{P/U}$	Transformed yield factor for $Y_{P/U}$.
ξ	Contact factor.
r_A	Rate of production of organism A in the first stage.
r_B, r_C	Rates of production of organisms B and C respectively in the second stage.
r_S	Rate of consumption of substrate S in the first stage.
r_{R_1}, r_{U_1}	Rates of consumption of organics R and U respectively in the first stage.
r_{R_2}, r_{U_2}	Rates of consumption of organics R and U respectively in the second stage.
r_P	Rate of production of product P in the second stage.
J	Objective function.
z_S, z_R, z_U	Penealization for discharging organics S, R, and U respectively.
Σ	Response surface.
A	Minimum point on (Σ).
B, D	Saddle points on (Σ).
C	Maximum point on (Σ).
h_{ij}	Hessian matrix.

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COMPUTER PROGRAM

Main routine MICU20 and subroutines

```
C MAIN PROGRAM MICU20.
C THIS PROGRAM DEFINES THE OPTIMAL DESIGN OF A TWO-STAGE WATER TREATMENT
C BY MIXED CULTURES. IT CALLS 4 SUBROUTINES SIMPLE,OBJ,NEWTON,ISOBAT
C                                  1 FUNCTION    QUART
C PROGRAMMER   JC DALTES                       KSU,MANHATTAN,FALL 68
C
C FIRST PART*****APECIFICATIONS, STATEMENT FUNCTION DEFINITIONS AND DATA
C                READING.
      EXTERNAL OBJ
      REAL KA,KS,KB,KR,KC,KU,MUS,MUR,MUU,KBO,KCO
      DIMENSION TITLE(30),TH(2,3),TMIN(2),DV(2)
      COMMON THW1,THW2,THW3,MUS,MUR,MUU,KA,KS,KB,KC,KU.DELTS,DELTAY
      COMMON /SEARCH/NDIM,KDIM,TH,ALPHA,BETA,GAMMA,IBARY,EPSIL,LIMIT,
     1                ICONV,TMIN,SMIN,NITER,CRIT,NEVAL
C
C READ AND ECHO-CHECK DATA. DEFINE STATEMENT FUNCTIONS.
      X1S1(T) = KS/(T*KA - 1.)
      DELTAS(T)= X1SO - X1S1(T)
      X2A1(T)= YAS*DELTAS(T)
      X1R1(T)= YRS*DELTAS(T)
      X1U1(T)= YUS*DELTAS(T)
      X1R2(T)= KR/(T*KB - 1.)
      DELTAR(T,U)= X1R1(T)-X1R2(U)
      X1U2(U) = KU/(U*KC-1.)
      DELTAU(T,U) = X1U1(T) - X1U2(U)
      X2B2(T,U) = YBR*DELTAR(T,U)
      X2C2(T,U) = YCU*DELTAU(T,U)
      X1P2(T,U) = YPR/YBR*X2B2(T,U) + YPU/YCU*X2C2(T,U)
      W2(T1)= (KR+X1R1(T1))/(KB*X1R1(T1))
      W3(T1)= (KU+X1U1(T1))/(KC*X1U1(T1))
      READ(1,1010)  TITLE
      WRITE(3,3010) TITLE
      READ(1,1020) X1SO,KA,KS,YAS,YRS,YUS
      WRITE(3,3020)X1SO,KA,KS,YAS,YRS,YUS
      READ(1,1020) KSO,KR,YBRO,YPRO
      WRITE(3,3030)KBO,KR,YBRO,YPRO
      READ(1,1020) KCO,KU,YCUO,YPUO
      WRITE(3,3040)KCO,KU,YCUO,YPUO
      READ(1,1020)      MUS,MUR,MUU
      WRITE(3,3081)     MUS,MUR,MUU
      PARAM=0
    5 READ(1,1020,END=85) R,BET
      CONTAC= 1.-(BET-1.)*R
      WRITE(3,3075) R,BET,CONTAC
      IF(CONTAC.GT.0.0) GO TO 10
      WRITE(3,3076)
      STOP
C
C GENERATE FICTITIOUS CONSTANTS FOR THE SECOND STAGE.
   10 KB=KBO/CONTAC
      KC=KCO/CONTAC
      YBR=YBRO/CONTAC
      YCU=YCUO/CONTAC
```

```
      YPR=YPRO/(1.+R)
      YPU=YPUO/(1.+R)
      WRITE(3,3077) KB,KC,YBR,YCU,YPR,YPU
      THW1= (KS+X1SO)/(KA*X1SO)
      IF(PARAM.EQ.1) GO TO 12
      IF(NOPT.EQ.0) GO TO 25
C
C IF OPTIMIZATION PROBLEM, READ IN AND WRITE PARAMETERS FOR SEARCH.
      WRITE(3,3083)
      NDIM=2
      KDIM=NDIM+1
      WRITE(3,3050)NDIM
      READ(1,1070) ALPHA,DETA,GAMMA,STEP,IBARY
      WRITE(3,3061)
      WRITE(3,3070)ALPHA,BETA,GAMMA,STEP,IBARY
      READ(1,1080) EPSIL,LIMIT,ETA,MAXIT
      WRITE(3,3080) ESPSIL,ETA
      WRITE(3,3082)
C
C SECOND PART*****DELTERMINATION OF OPTIMAL POLICY
C DIFFERNTIAL CALCULUS APPROACH.
   12 WRITE(3,3085)
      TH1OPT=1./KA*(1.+SQRT(MUS*KS*KA))
      TEST1= MUS*KA*X1SO*X1SC - KS
      CALL NEWTON(TH2OPT)
      THW3=(KU+X1U1(TH1OPT))/(KC*X1U1(TH1OPT))
      TEST2= QUART(THW3)
      WRITE(3,3086) TH1OPT,TEST1,TH2OPT,TEST2
      IF(TEST1.GT.0.0.AND.TEST2.GT.0.0) GO TO 15
      WRITE(3,3088)
      STOP
C
C SEARCH TECHNIQUE APPROACH.
   15 WRITE(3,3087)
      LLAC=0
      NEVAL=0
      RTH1= TH1OPT+0.5
      RTH2= TH2OPT+1.
C
C ENTER OPTIMIZATION LOOP.
   21 TH(1,1)= TH1OPT+STEP
      TH(2,1)= TH2OPT
      TH(1,2)= TH1OPT
      TH(2,2)= TH2OPT+STEP
      TH(1,3)= TH1OPT+STEP
      TH(2,3)= TH2OPT+STEP
      THW2= W2(RTH1)
      THW3= W3(RTH1)
      CALL SIMPLE(OBJ)
      LLAC=LLAC+1
      IF(ICONV.EQ.1) GO TO 22
      WRITE(3,3150) NITER,CRIT
      STOP
```

```
   22 IF(ABS(TMIN(1)-RTH1).LT.ETA.AND.ABS(TMIN(2)-RTH2).LT.ETA) GO TO 23
      IF(LLAC.EQ.MAXIT) GO TO 24
      RTH1=TMIN(1)
      RTH2=TMIN(2)
      GO TO 21
   24 WRITE(3,3100) LLAC
      STOP
   23 RT1= TMIN(1)
      RT2= TMIN(2)
      THW2= W2(RT1)
      THW3= W3(RT1)
      WRITE(3,3109) LLAC
      WRITE(3,3110) RT1,RT2
      WRITE(3,3140) SMIN
      GO TO 26
C
C THIRD PART*****THE POLICY IS FIXED BY THE USER WITHOUT BEING OPTIMAL.
C IF NO OPTIMIZATION PROBLEM
   25 WRITE(3,3084)
      READ(1,1020,END=999) RT1,RT2
      WRITE(3,3042) RT1,RT2
      DV(1)= RT1
      DV(2)= RT2
      THW2= W2(RT1)
      THW3= W3(RT1)
      NEVAL=0
      WRITE(3,3082)
      CALL OBJ(DV,S)
      WRITE(3,3490) S
C
C FOURTH PART***** STATE CORRESPONDING TO THE CHOSEN POLICY
   26 WRITE(3,3500) THW1,RT1
      IF(RT1.GT.THW1) GO TO 34
   30 WRITE(3,3079)
      STOP
   34 S1= X1S1(RT1)
      A1= X2A1(RT1)
      R1= X1R1(RT1)
      U1= X1U1(RT1)
      WRITE(3,3120) S1,A1,R1,U1
      WRITE(3,3520) THW2,THE3,RT2
      IF(RT2.GT.THW3) GO TO 35
      GO TO 30
   35 R2= X1R2(RT2)
      U2= X1U2(RT2)
      B2= X2B2(RT1,RT2)
      C2= X2C2(RT1,RT2)
      P2= X1P2(RT1,RT2)
      WRITE(3,3130) R2,U2,B2,C2,P2
      SRT= RT2/CONTAC
      WRITE(3,3089) SRT
      IF(ICURV.EQ.0) GO TO 75
C
```

```
C FIFTH PART ***** OUTPUT OF CURVES CORRESPONDING TO THE CHOSEN POLICY.
C     1) FIRST STAGE
   36 WRITE(3,3180)
      S1= X1S1(THW1)
      A1= X2A1(THW1)
      R1= X1R1(THW1)
      U1= X1U1(THW1)
      DX1S1= -KS*KA/(KA*THW1-1.)**2
      DX2A1= -YAS*DX1S1
      DX1R1= -YRS*DX1S1
      DX1U1= -YUS*DX1S1
      WRITE(3,3190) THW1,S1,A1,R1,U1,DX1S1,DX2A1,DX1R1,DX1U1
      RT = (AINT(10.*THW1)+1.)/10
   40 S1= X1S1(RT)
      A1= X2A1(RT)
      R1= X1R1(RT)
      U1= X1U1(RT)
      WRITE(3,3190) RT,S1,A1,R1,U1
      RT= RT+0.1
      DIF= RT - AINT(RT)
      IF(.NOT.(1.-DIF.LT.0.01.OR.DIF.LT.0.01)) GO TO 40
   50 S1= X1S1(RT)
      A1= X2A1(RT)
      R1= X1R1(RT)
      U1= X1U1(RT)
      WRITE(3,3190) RT,S1,A1,R1,U1
      RT=RT+1.
      IF(RT.LE.20.0) GO TO 50
C
C     2) SECOND STAGE BETWEEN THW2 AND THW3.
      WRITE(3,3200)
      R2= X1R2(THW2)
      B2= X2B2(RT1,THW2)
      P2= YPR/YBR*B2
      DX1R2= -KR*KB/(THW2*KB-1.)**2
      DX2B2= -YBR*DX1R2
      D1X1P2= YPR/YBR*DX2B2
      WRITE(3,3210) THW2,R2,B2,P2,DX1R2,DX2B2,D1X1P2
      RT= (AINT(10.*THW2)+1.)/10
   60 R2= X1R2(RT)
      B2= X2B2(RT1,RT)
      P2= YPR/YBR*B2
      WRITE(3,3210) RT,R2,B2,P2
      RT=RT+0.1
      DIF= RT - AINT(RT)
      IF(.NOT.(1.-DIF.LT.0.01.OR.DIF.LT.0.01)) GO TO 60
   61 R2= X1R2(RT)
      B2= X2B2(RT1,RT)
      P2= YPR/YBR*B2
      WRITE(3,3210) RT,R2,B2,P2
      RT=RT+1.
      IF(RT.GE.THW3) GO TO 71
      GO TO 61
```

```
C
C      3) SECOND STAGE ABOVE THW3
   71 WRITE(3,3220)
      R2= X1R2(THW3)
      B2= X2B2(RT1,THW3)
      P2= X1P2(RT1,THW3)
      U2= X1U2(THW3)
      C2= X2C2(RT1,THW3)
      DX1U2= -KU*KC/(THW3*KC-1.)**2
      DX2C2= -YCU*DX1U2
      D2X1P2= YPR*KR*KC/(KB*THW3-1.)**2
      D3X1P2= YPU/YCU*DX2C2+D2X1P2
      WRITE(3,3230) THW3,R2,B2,P2,U2,C2,DX1U2,DX2C2,D2X1P2,D3X1P2
      RT= (AINT(10.*THW3)+1.)/10
   73 R2= X1R2(RT)
      B2= X2B2(RT1,RT)
      P2= X1P2(RT1,RT)
      U2= X1U2(RT)
      C2= X2C2(RT1,RT)
      WRITE(3,3230) RT,R2,B2,P2,U2,C2
      RT=RT+0.1
      DIF=RT-AINT(RT)
      IF(.NOT.(1.-DIF.LT.0.01.OR.DIF.LT.0.01)) GO TO 73
   72 R2= X1R2(RT)
      B2= X2B2(RT1,RT)
      P2= X1P2(RT1,RT)
      U2= X1U2(RT)
      C2= X2C2(RT1,RT)
      WRITE(3,3230) RT,R2,B2,P2,U2,C2
      RT=RT+1.
      IF(RT.LE.20.) GO TO 72
   75 IF(ICONT.NE.0) GO TO 80
      PARAM=1
      GO TO 5
C
C SIXTH PART ***** DRAW THE CONTOURS OF THE OBJECTIVE FUNCTION.
   80 READ(1,1020) DELTS,DELTAY
      CALL ISOBAT
   85 WRITE(3,3240)
      GO TO 1000
  999 WRITE(3,3540)
 1000 STOP
 1010 FORMAT(20A4/10A4)
 1020 FORMAT(6F10.0)
 1041 FORMAT(3I10)
 1070 FORMAT(4F10.0,I10)
 1080 FORMAT(2(E10.2,110))
 3010 FORMAT(I10,30A4////T55,5H*****/T55,6H*DATA*/T55,5H*****//)
 3020 FORMAT(19H FEED CONCENTRATION,21X,4HX1SO,F9.2,5H GM/L/
     1       29H MAXIMUM SPECIFIC GROWTH RATE,11X,2HKA,F11.2,6H DAY-1/
     2       20H SATURATION CONSTANT,20X,2HKS,F11.2,5H GM/L/
     3       14H YIELD FACTORS,26X,3HYAS,F10.2/
     4       40X,3HYRS,F10.2/
```

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    5          40X,3HYUS,F10.2//)
3030 FORMAT(29H MAXIMUM SPECIFIC GROWTH RATE,11X,2HKB,F11.2,6H DAY-1/
    1          20H SATURATION CONSTANT,20X,2HKR,F11.2,5H GM/L/
    2          14H YIELD FACTORS,26X,3HYBR,F10.2/
    3          40X,3HYPR,F10.2//)
3040 FORMAT(29H MAXIMUM SPECIFIC GROWTH RATE,11X,2HKC,F11.2,6H DAY-1/
    1          20H SATURATION CONSTANT,20X,2HKU,F11.2,5H GM/L/
    2          14H YIELD FACTORS,26X,3HYCU,F10.2/
    3          40X,3HYPU,F10.2//)
3042 FORMAT(16H RESIDENCE TIMES,24X,3HRT1,F10.2/
    1          40X,3HRT2,F10.2/)
3050 FORMAT(18H SEARCH PARAMETERS/15HODIMENSIONALITY,25X,4HNDIM,I6/)
3061 FORMAT(9H STRATEGY/)
3070 FORMAT(11H REFLECTION,29X,5HALPHA,F8.2/
    1          12H CONTRACTION 28X,4HBETA,F9.2/
    2          10H EXPANXION 30X,5HGAMMA,F8.2/
    3          T41,'STEP',F9.2/T41,5HIBARY,I5/)
3075 FORMAT('1RECYCLE RATIO',T41,'R',F13.3/
    1          'CLARIFYER EFFICIENCY',T41,'BET',F11.3/
    2          'CONTACT FACTOR',T41,'CONTAC',F8.3//)
3076 FORMAT('1THE CONTACT FACTOR IS NOT POSITIVE.'//)
3077 FORMAT('FICTITIOUS CONSTANTS: KB/KC/YBR/YCU/YPR/YPU',6F10.2//)
3079 FORMAT('OTHIS POLICY IS NOT FEASIBLE'///)
3080 FORMAT(20H PRESCRIBED ACCURACY,20X,5HEPSIL,1PE11.1/
    1          33H ACCURACY OF OVER ALL CONVERGENCE,7X,3HETA,1PE13.1/)
3081 FORMAT(31H PENALIZATION FOR DISCHARGING S,9X,3HMUS,F12.4/
    1          30X,1HR,9X,3HMUR,F12.4/
    2          30X,1HU,9X,3HMUU,F12.4//)
3082 FORMAT(1H1,T56,9H*********/T56,9H*RESULTS*/T56,9H*********///
    1          47H CONCENTRATIONS ARE IN GM/L. TIMES ARE IN DAYS.///)
3083 FORMAT(36HODETERMINATION OF THE OPTIMAL POLICY///)
3084 FORMAT(33HOTHE CHOSEN POLICY IS NOT OPTIMAL/
    1          33H*********************************)
3085 FORMAT(46X,6H***** 14HOPTIMAL POLICY 6H *****//
    1          45X,30HDIFFERENTIAL CALCULUS APPROACH//)
3086 FORMAT(1H 39X,6HTH1OPT,1PE12.3/1H 39X,5HTEST1,1PE12.2//
    1          1H 39X,6HTH2OPT,1PE12.3/40X,5HTEST2,1PE12.2//)
3087 FORMAT(50X,16HSIMPLEX APPROACH//)
3088 FORMAT('1NEGATIVE TEST FOR FEASIBILITY. THE CALCULATIONS ARE',
    1          ' STOPPED'//)
3089 FORMAT(///' SOLID RETENTION TIME IN SECOND STAGE',
    1          T41,'SRT',F11.3//)
3100 FORMAT(31H CALCULATIONS ARE STOPPED AFTER,I5,12H ITERATIONS.)
3109 FORMAT(35H CONVERGENCE HAS BEEN REACHED AFTER,I4,11H ITERATIONS/)
3110 FORMAT(27H OPTIMAL DECISION VARIABLES,1PE31.3/1H 1PE57.3/)
    1          40X,4HX2A1,F10.3/40X,4HX1R1,F10.3/40X,4HX1U1,F10.3/)
3130 FORMAT(33H STATE VECTOR AT THE SECOND STAGE,7X,4HX1R2.F10.3/
    1          40X,4HX1U2,F10.3/40X,4HX2B2,F10.3/40X,4HX2C2,F10.3/
    2          40X,4HX1P2,F10.3/)
3140 FORMAT(27H OPTIMAL OBJECTIVE FUNCTION,1PE32.4/)
3150 FORMAT(6H AFTER,I5,33H ITERATIONS, THE CRITERION EQUALS 1PE10.2/
    1   26H CALCULATIONS ARE STOPPED./)
```

```
3180 FORMAT(1H1,43X,6H***** 20HCONCENTRATION CURVES 6H *****/////
    1        55X,11HFIRST STAGE///
    1        5X,2HTH,10X,4HX1S1,11X,4HX2A1,11X,4HX1R1,
    2 11X,4HX1U1,10X,5HDX1S1,10X,5HDX2A1,10X,5HDX1R1,10X,5HDX1U1/)
3190 FORMAT(F8.3,F13.3,7F15.3)
3200 FORMAT(1H1,45X,34HSECOND STAGE BETWEEN THW2 AND THW3////
    1        4X,2HTH,10X,4HX1R2,
    2 11X,4HX2B2,11X,4HX1P2,10X,5HDX1R2,10X,5HDX2B2,10X,6HD1X1P2/)
3210 FORMAT(F7.3,F14.3,5F15.3)
3220 FORMAT(1H1,50X,23HSECOND STAGE ABOVE THW3////
    1        4X,2HTH,10X,4HX1R2,11X,4HX2B2,
    2        11X,4HX1P2,11X,4HX1U2,12X,4HX2C2, 7X,5HDX1U2, 7X,5HDX2C2, 6X,
    3 6HD2X1P2,6X,6HD3X1P2//)
3230 FORMAT(F7.3,F14.3,4F15.3,4F12.3)
3240 FORMAT(19H1NORMAL TERMINATION)
3490 FORMAT(19H OBJECTIVE FUNCTION,F35.3/)
3500 FORMAT(1H0,52X,11HFIRST STAGE//14H WASH OUT TIME,F40.3//
    1  15H RESIDENCE TIME,F39.3/)
3520 FORMAT(1H0,52X12HSECOND STAGE//15H WASH OUT TIMES,F39.3/
    1        1H F53.3//15H RESIDENCE TIME,F39.3/)
3540 FORMAT( 31H1NO RESIDENCE TIMES FOUND. STOP)
     END
```

```
      SUBROUTINE SIMPLE(OBJ)
C THIS SUBROUTINE FINDS THE MINIMUM OF THE OBJECTIVE FUNCTION GIVEN
C BY SUBROUTINE OBJ. THE ARGUMENT OF SIMPLE REQUIRES AN EXTERNAL
C STATEMENT IN THE CALLING ROUTINE.
C FOLLOWING VARIABLES SHOULD BE PREVIOUSLY DEFINED AND STORED IN
C COMMON /SEARCH/
C NDIM,KDIM,TH,ALPHA,BETA,GAMMA,IBARY,EPSIL,LIMIT
C THIS S.NE DEFINES AND STORES INTO THE SAME AREA
C ICONV,TMIN,SMIN,NITER,CRIT WHERE TMIN IS THE OPTIMAL DECISION BECTOR.
C NEVAL IS DEFINED BY S.NE OBJ.
C IF THE SEARCH CONVERGED, ICONV=1. IF NOT, ICONV=-1 AND THE BEST
C CURRENT POINT IS CONSIDERED AS OPTIMAL.
C DIMENSIONS    T,SIGTH,TBAR,TREF,TEXP,TCON,TMIN      NDIM
C               S,W                                   KDIM
C               TH                                    NDIM,KDIM
C CHANGING THE DIMENSIONALITY OF THE SEARCH REQUIRES THE PROPER
C DIMENSION STATEMENT. THIS SUBROUTINE HAS BEEN TESTED FOR NDIM=1,2,3,4,20.
C PROGRAMMER JC BALTES                           KSU, CHEM ENG, FEB 68
C
C SPECIFICATIONS.
      COMMON /SEARCH/NDIM,KDIM,TH,ALPHA,BETA,GAMMA,IBARY,EPSIL,LIMIT,
     1               ICONV,TMIN,SMIN,NITER,CRIT,NEVAL
      DIMENSION TH(2,3),T(2),S(3),SIGTH(2),TBAR(2),TREE(2),TEXP(2),
     1          TCON(2),TMIN(2),W(3)
C
C INITIALIZATION
      NITER=0
      ICONV=0
C
C COMPUTE INITIAL FUNCTION VALUES.
      DO 30 J=1,KDIM
      DO 40 I=1,NDIM
   40 T(I)=TH(I,J)
   30 CALL OBJ(T,S(J))
C
C BEGINNING OF ITERATIONS.
C DEFINE THE POINT HAVING THE HIGHEST FUNCTION VALUE
   41 SH = S(1)
      JH=1
      DO 50 J=2,KDIM
      IF(S(J).LE.SH) GO TO 50
      SH=S(J)
      JH=J
   50 CONTINUE
C
C DEFINE THE POINT HAVING THE LOWEST VALUE OF THE OBJECTIVE FUNCTION.
   51 SL=S(1)
      JI=1
      DO 60 J=2,KDIM
      IF(S(J).GE.SL) GO TO 60
      SL=S(J)
      JI=J
   60 CONTINUE
```

```
      IF(ICONV*ICONV.EQ.1) GO TO 320
C
C DETERMINATION OF THE CENTROID
      IF(IBARY.NE.0) GO TO 90
      DO 70 I=1,NDIM
      SIGTH(I)=0.
      DO 80 J=1,KDIM
      IF(J.EQ.JH) GO TO 80
      SIGTH(I)=SIGTH(I)+TH(I,J)
   80 CONTINUE
   70 TBAR(I)=SIGTH(I)/FLOAT(NDIM)
      GO TO 130
   90 SIGMAW=0.
      DO 100 J=1,KDIM
      W(J)=S(JH)-S(J)
  100 SIGMAW=SIGMAW+W(J)
      DO 110 I=1,NDIM
      SIGTH(I)=0.
      DO 120 J=1,KDIM
  120 SIGTH(I)=SIGTH(I)+W(J)*TH(I,J)
  110 TBAR(I)=SIGTH(I)/SIGMAW
  130 CALL OBJ(TBAR,SBAR)
C
C REFLECTION GIVES POINT (TREF)
      DO 140 I=1,NDIM
  140 TREF(I)= (1.+ALPHA)*TBAR(I)-ALPHA*TH(I,JH)
      CALL OBJ(TREF,SREF)
      IF (SREF.LT.S(JL)) GO TO 160
      DO 150 J=1,KDIM
      IF(J.EQ.JH) GO TO 150
      IF (STREF.GT.S(J)) GO TO 150
      GO TO 180
  150 CONTINUE
      GO TO 220
C
C EXPANSION GIVES POINT (TEXP)
  160 DO 170 I=1,NDIM
  170 TEXP(I)= GAMMA*TREF(I) + (1.-GAMMA)*TBAR(I)
      CALL OBJ(TEXP,SEXP)
      IF(SEXP.LT.S(JL)) GO TO 200
  180 DO 190 I=1,NDIM
  190 TH(I,JH)=TREF(I)
      S(JH)=SREF
      GO TO 300
  200 DO 210 I=1,NDIM
  210 TH(I,JH)=TEXP(I)
      S(JH)=SEXP
      GO TO300
C
C CONTRACTION GIVES POINT (TCON)
  220 IF(SREF.GT.S(JH)) GO TO 240
      DO 230 I=1,NDIM
  230 TH(I,JH)=TREF(I)
```

```
  240 DO 250 I=1,NDIM
  250 TCON(I)=BETA*TH(I,JH) + (1.- BETA)*TBAR(I)
      CALL OBJ(TCON,SCON)
      IF(SCON.GT.S(JH)) GO TO 270
      DO 260 I=1,NDIM
  260 TH(I,JH)=TCON(I)
      S(JH)=SCON
      GO TO 300
  270 DO 290 J=1,KDIM
      IF(J.EQ.JL) GO TO 290
      DO 250 I=1,NDIM
      TH(I,J)= (TH(I,J)+TH(I,JL)0/FLOAT(NDIM)
  280 T(I)=TH(I,J)
      CALL OBJ(T,S(J))
  290 CONTINUE
C
C CRITERION FOR CONVERGENCE.
  300 SQDELS=0.
      DO 310 J=1,KDIM
  310 SQDELS=SQDELS+(S(J)-SBAR)**2
      CRIT=SQRT(SQDELS/FLOAT(NDIM)
      NITER=NITER+1
      IF(CRIT.GE.EPSIL) GO TO340
      ICONV=1
      GO TO 51
  340 IF(NITER.LT.LIMIT) GO TO 41
      ICONV=-1
      WRITE(3,3010) NITER
 3010 FORMAT(49H1THE SEARCH RETURNS THE BEST CURRENT POINT AFTER,
     1       12HITERATION NO 15,31H. THIS IS NOT THE TRUE OPTIMUM.//)
      GO TO 51
  320 DO 330 I=1,NDIM
  330 TMIN(I)=TH(I,JL)
      SMIN=S(JL)
      RETURN
      END
```

```
FUNCTION QUAR(U)
REAL KA,KS,KB,KR,KC,KU,MUS,MUR,MUU
COMMON THW1,THW2,THW3,MUS,MUR,MUU,KA,KS,KB,KR,KC,KU,DELTS,DELTAY
QUART   =  MUR*KR*KB/(U*KB-1.)**2 + MUU*KU*KC/(U*KC-1.0**2-1.
RETURN
END
```

```
      SUBROUTINE NEWTON(ROOT)
C
C THIS SUBROUTINE COMPUTES A ROOT OF QUART=0
      REAL KA,KS,KB,KR,KC,KU,MUS,MUR,MUU
      COMMON THW1,THW2,THW3,MUS,MUR,MUU,KA,KS,KB,KR,KC,KU,DELTS,DELTAY
      DQUART(U)= -2.*MUR*KR*KB*KB/(U*KB-1.)**3
     1         -2.*MUU*KU*KC**2/(U*KC-1.0**3
C
C LOOK FOR AN INTERVAL WHERE FUNCTION QUART HAS OPPOSITE SIGNS.
      X1= 1./KC+0.01
    5 X2= X1+0.10
      IF(QUART(X1)*QUART(X2).LE.0.0) GO TO 10
      X1=X2
      GO TO 5
C
   10 X2= X1 -(QUART(X1)/DQUART(X1))
      IF(ABS(X1-X2).LT.1.0E-04) GO TO 20
      X1=X2
      GO TO 10
   20 ROOT=X2
      RETURN
      END
```

```
      SUBROUTINE OBJ(T,S)
      REAL KA,KS,KB,KR,KC,KU,MUS,MUR,MUU
      COMMON THW1,THW2,THW3,MUS,MUR,MUU,KA,KS,KB,KR,KC,KU,DELTS,DELTAY
      COMMON /SEARCH/ BICON(20),NEVAL
      DIMENSION T(1)
C
      IF(T(1).LT.THW1.OR.T(2).LT.THW3) GO TO 10
      X1S2= KS/(KA*T(1)-1.)
      X1R2= KR/(KB*T(2)-1.)
      X1U2= KU/(KC*T(2)-1.)
      S=     (T(1)+T(2)) + MUS*X1S2 + MUR*X1R2 + MUU*X1U2
      NEVAL= NEVAL+1
      GO TO 20
   10 S= 1.0E+06
   20 RETURN
      END
```

```
      SUBROUTINE ISOBAT
C
C SPECIFICATIONS.
      REAL KA,KS,KB,KR.KC,KU,MUS,MUR,MUU
      INTEGER S110
      DIMENSION TITLE(30),TH(2,3),TMIN(2).DV(2)
      COMMON THW1,THW2,THW3,MUS,MUR,MUU,KA,KS,KB,KR,KC,KU,DELTS,DELTAY
      COMMON /SEARCH/NDIM,KDIM,TH,ALPHA,BETA,GAMMA,IBARY,EPSIL,LIMIT,
     1                ICONV,TMIN,SMIN,NITER,CRIT,NEVAL
C
      WRITE(3,3240)
      S=  (AINT(10.*SMIN)+1.)/10.
      S110=0
   76 DO 110 I=1,10
      WRITE(3,3250) S
C
C INCREASE Y.
      Y= (AINT(TMIN(2)*10.)+1.)/10
      DO 80 J=1,25
      IF(ABS(Y-1./KB).LT.1.OE-04.OR.ABS(Y-1./KC).LT.1.OE-04) GO TO 79
      A= Y+MUR*KR/(KB*Y-1.) + MUU*KU/(KC*Y-1.)
      DISCR= ((A-S)*KA-1.)**2 -4.*KA*(MUS*KS+S-A)
      IF(DISCR.LT.O.) GO TO 81
      X1= (1.-(A-S)*KA + SQRT(DISCR))/(2.*KA)
      X2= (1.-(A-S)*KA - SQRT(DISCR))/(2.*KA)
      WRITE(3,3260)X1,X2,Y
   79 Y=Y+DELTAY
   80 CONTINUE
C
C DECREASE Y.
   81 Y= (AINT(TMIN(2)*10.))/10.
      DO 90 J=1,20
      IF(ABS(Y-1./KB).LT.1.OE-04.OR.ABS*Y-1./KC).LT.1.OE-04) GO TO 89
      A= Y+MUR*KR/(KB*Y-1.) + MUU*KU/(KC*Y-1.)
      DISCR= ((A-S)*KA-1.)**2 -4.*KA*(MUS*KS+S-A)
      IF(DISCR.LT.O.) GO TO 100
      X1= (1.-(A-S)*KA + SQRT(DISCR))/(2.*KA)
      X2= (1.-(A-S)*KA - SQRT(DISCR))/(2.*KA)
      WRITE(3,3260) X1,X2,Y
   89 Y=Y-DELTAY
   90 CONTINUE
  100 S=S+DELTS
      IF(S110.EQ.1) RETURN
  110 CONTINUE
      S110=1
      S=1.10*SMIN
      WRITE(3,3251)
      GO TO 76
 3240 FORMAT(1H1,49X,6H***** 8HCONTOURS 6H *****//)
 3250 FORMAT(19HOOBJECTIVE FUNCTION,F12.2,4X,2HX1,8X,2HX2,8X,1HY/)
 3251 FORMAT( 34HOCONTOUR CORRESPONDING TO 1.1*SMIN)
 3260 FORMAT(1H ,F38.3,2F10.3)
      END
```

APPENDIX I

SLOPE OF THE CONCENTRATION CURVES AT THE POINTS OF DISCONTINUITY

At the points of discontinuity of the concentration curves, wash-out occurs for organism A, B or C. In order to draw these curves with accuracy, it is useful to determine their slopes at the wash-out residence times θ_{w1}, θ_{w2}, and θ_{w3}.

In the first stage, wash-out occurs when $\theta_1 = \theta_{w1}$. Then, from equations (12), (14), (16) and (17), we obtain respectively

$$\left.\frac{dS_1}{d\theta_1}\right|_{\theta_{w1}} = \frac{-K_S\, k_A}{(k_A\, \theta_{w1} - 1)^2}$$

$$\left.\frac{dA}{d\theta_1}\right|_{\theta_{w1}} = - Y_{A/S} \left.\frac{dS_1}{d\theta_1}\right|_{\theta_{w1}}$$

$$\left.\frac{dR_1}{d\theta_1}\right|_{\theta_{w1}} = - Y_{R/S} \left.\frac{dS_1}{d\theta_1}\right|_{\theta_{w1}}$$

$$\left.\frac{dU_1}{d\theta_1}\right|_{\theta_{w1}} = - Y_{U/S} \left.\frac{dS_1}{d\theta_1}\right|_{\theta_{w1}}$$

In the second stage, wash-out occurs for organism B and C when $0 < \theta_2 \leq \theta_{w2}$. When $\theta_{w2} < \theta_2 \leq \theta_{w3}$, organism B alone grows using organics R and yielding product P. Then, from equations (19), (24), and (27), we obtain respectively

$$\left.\frac{dR_2}{d\theta_2}\right|_{\theta_{w2}} = - \frac{K_R\, k_B}{(k_B\, \theta_{w2} - 1)^2}$$

$$\left.\frac{dB}{d\theta_2}\right|_{\theta_{w2}} = - Y_{B/R} \left.\frac{dR_2}{d\theta_2}\right|_{\theta_{w2}}$$

and

$$\left.\frac{dP}{d\theta_2}\right|_{\theta_{w2}} = \frac{Y_{P/R}}{Y_{B/R}} \cdot \left.\frac{dB}{d\theta_2}\right|_{\theta_{w2}}$$

$$\left.\frac{dP}{d\theta_2}\right|_{\theta_{w3-}} = \frac{Y_{P/R}}{Y_{B/R}} \left.\frac{dB}{d\theta_2}\right|_{\theta_{w3-}}$$

When $\theta_2 > \theta_{w3}$, both organisms B and C grow. Concentration U_2 falls, yielding more product P. From equations (20), (25), and (27), we obtain respectively

$$\left.\frac{dU_2}{d\theta_2}\right|_{\theta_{w3}} = \frac{- K_U\ k_C}{(k_C\ \theta_{w3} - 1)^2}$$

$$\left.\frac{dC}{d\theta_2}\right|_{\theta_{w3+}} = - Y_{C/U} \left.\frac{dU_2}{d\theta_2}\right|_{\theta_{w3}}$$

$$\left.\frac{dP}{d\theta_2}\right|_{\theta_{w3+}} = \frac{Y_{P/R}}{Y_{B/R}} \cdot \left.\frac{dB}{d\theta_2}\right|_{\theta_{w3}} + \frac{Y_{P/U}}{Y_{C/U}} \cdot \left.\frac{dC}{d\theta_2}\right|_{\theta_{w3}}$$

APPENDIX II

GRAPHICAL DETERMINATION OF THE ROOTS OF EQUATION $\varphi(\theta_2) = 0$

Let us examine the function $\varphi(\theta_2)$ defined by equation (74). From this equation we can deduce that when $\theta_2 \to \pm\infty$, $\varphi \to -1$ and when $\theta_2 \to \frac{1}{k_B}$ or $\frac{1}{k_C}$, $\varphi \to +\infty$. The sign of the derivative $\frac{d\varphi}{d\theta_2}$ gives useful information about the function $\varphi(\theta_2)$. From equation (74), we obtain

$$\frac{d\varphi}{d\theta_2} = \frac{-\theta z_R K_R k_B^2}{(k_B\theta_2 - 1)^3} - \frac{2 z_U K_U k_C^2}{(k_C\theta_2 - 1)^3} \tag{87}$$

The abscissa of the stationary points of function $\varphi(\theta_2)$ are given by

$$\frac{d\varphi}{d\theta_2} = 0 \tag{88}$$

Employing the expression given by equation (87) and rearranging yields

$$\left(\frac{k_C\theta_2 - 1}{k_B\theta_2 - 1}\right)^3 = -\frac{z_U K_U k_C^2}{z_R K_R k_B^2}$$

Let

$$-\frac{z_U K_U k_C^2}{z_R K_R k_B^2} = -\rho^3 \quad \text{and} \quad \left(\frac{k_C\theta^2 - 1}{k_B\theta^2 - 1}\right)^3 = \Theta^3$$

Then

$$= \left(\frac{z_U\ K_U\ k_C}{z_R\ K_R\ k_B}\right)^{1/3} > 0$$

Solving equation (88) for stationary points of function $\varphi(\theta_2)$ gives

$$\Theta^3 + \rho^3 = 0 \tag{89}$$

which may be written as

$$(\Theta + \rho)(\Theta^2 - \rho\Theta + \rho^2) = 0$$

This equation breaks down into

$$\Theta + \rho = 0 \tag{90}$$

and

$$\Theta^2 - \rho\Theta + \rho^2 = 0 \tag{91}$$

Let us first consider equation (86). It is quadratic with respect to Θ. Its discriminant is

$$\rho^2 - 4\rho^2 = -3\rho^2 < 0$$

Therefore, equation (91) has no real roots. Solving equation (90) yields

$$\Theta = \frac{k_C\ \theta_2 - 1}{k_B\ \theta_2 - 1} = -\rho$$

Hence

$$\theta_2 \equiv \theta_{2m} = \frac{1 + \rho}{k_C + \rho\, k_B} \tag{92}$$

Let us compare θ_{2m} to $\frac{1}{k_B}$.

$$\theta_{2m} = \frac{1}{k_B}\left(\frac{1+\rho}{\frac{k_C}{k_B}+\rho}\right)$$

But $\frac{k_C}{k_B}$ is less than 1. Consequently

$$\theta_{2m} > \frac{1}{k_B}$$

Now, θ_{2m} can be written as

$$\theta_{2m} = \frac{1}{k_C}\left(\frac{1+\rho}{1+\frac{k_B}{k_C}\rho}\right)$$

which shows immediately that

$$\theta_{2m} < \frac{1}{k_C}$$

Therefore, we have

$$\frac{1}{k_B} < \theta_{2m} < \frac{1}{k_C}\ .$$

It can thus be concluded that derivative $\frac{d\varphi}{d\theta_2}$ vanishes once in the interval $(-\infty, +\infty)$ for $\theta_2 = \theta_{2m}$. In addition, θ_{2m} lies between $\frac{1}{k_B}$ and $\frac{1}{k_C}$. Equation (53) gives the following additional information.

$$\text{when } \theta_2 \to \pm\infty, \qquad \frac{d\varphi}{d\theta_2} \to 0\pm$$

$$\text{when } \theta_2 \to \frac{1}{k_B} \pm 0, \quad \frac{d\varphi}{d\theta_2} \to \mp\infty$$

$$\text{when } \theta_2 \to \frac{1}{k_C} \pm 0, \quad \frac{d\varphi}{d\theta_2} \to \mp \infty$$

With this information we can set up the table for the variation of function $\varphi(\theta_2)$ (see Table 1). The numerical values which appear in the second part of Table 1 are computed from the numerical data given in Paragraph (IV. 2). θ_{2m} turns out to be the abscissa of a minimum for the graph of function $\varphi(\theta_2)$ (see Figure 19).

$$\theta_{2m} = \frac{1 + \rho}{k_C + \rho k_B}$$

$$\rho = \sqrt[3]{\left(\frac{1.50}{1.50}\right)\left(\frac{1.50}{1.00}\right)\left(\frac{0.25}{0.50}\right)^2}$$

$$= \sqrt[3]{0.375}$$

$$\rho = 0.720$$

$$\theta_{2m} = \frac{1 + 0.720}{0.25 + 0.720 \times 0.50} = \frac{1.720}{0.610}$$

Thus

$$\theta_{2m} = + 2.82$$

and the value of function φ is computed as follows;

$$\varphi(\theta_{2m}) = \frac{1.50 \times 1.00 \times 0.50}{(0.50 \times 2.82 - 1)^2}$$

$$+ \frac{1.50 \times 1.50 \times 0.25}{(0.25 \times 2.82 - 1)^2}$$

$$= \frac{1.750}{0.168} + \frac{0.563}{0.087} - 1$$

$$= 4.46 + 6.46 - 1$$

$$\varphi(\theta_{2m}) = + 9.92.$$

TABLE 1

VARIATIONS OF FUNCTION $\varphi(\theta^2)$

θ_2	$-\infty$		$\frac{1}{k_B}$		θ_m		$\frac{1}{k_C}$		$+\infty$
$\frac{d\varphi}{d\theta_2}$	0.	+	$+\infty$ ‖ $-\infty$	−	0	+	$+\infty$ ‖ $-\infty$	−	0
φ	−1	$\nearrow$	$+\infty$ ‖ $+\infty$	$\searrow$	$\varphi(\theta_m^2)$	$\nearrow$	$+\infty$ ‖ $-\infty$	$\searrow$	− 1

θ_2	$-\infty$		2		2.82		4		$+\infty$
$\frac{d\varphi}{d\theta_2}$	0	+	$+\infty$ ‖ $-\infty$	−	0	+	$+\infty$ ‖ $-\infty$	−	0
φ	−1	$\nearrow$	$+\infty$ ‖ $+\infty$	$\searrow$	+9.92	$\nearrow$	$+\infty$ ‖ $+\infty$	$\searrow$	−1

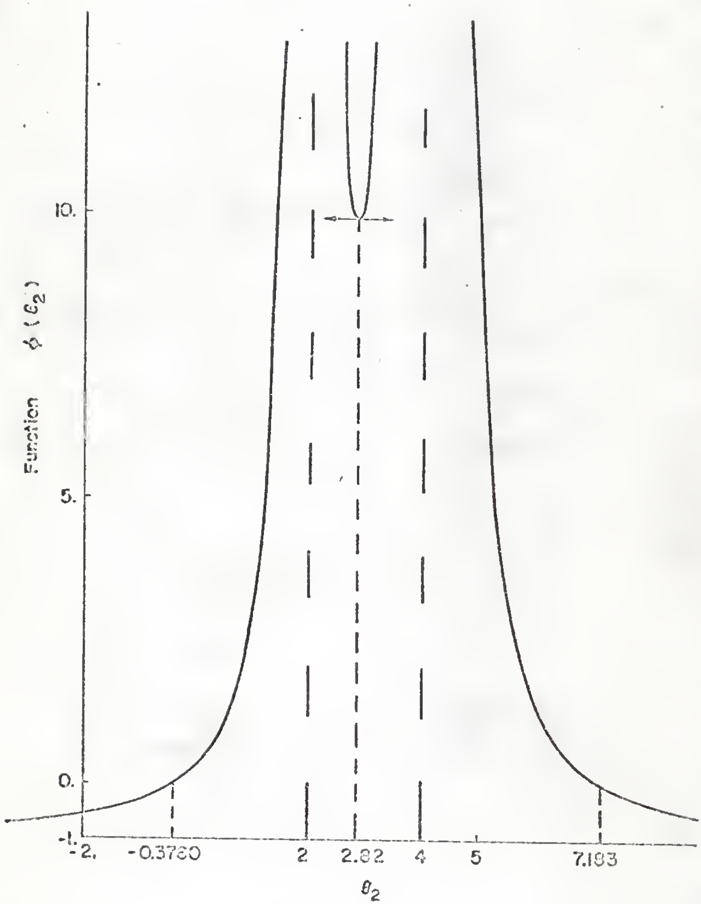

Fig. 19 Function $\phi(\theta_2)$.

Function $\varphi(\theta_2)$ is shown on Figure 19. Its graph intersects the θ_2 - axis at two points. Therefore, equation (73) has two real roots. The negative root is

$$\theta_2 = - 0.376$$

The positive root is

$$\theta_2 = + 7.183$$

Although $\theta_2 = -0.376$ is the ordinate of two stationary points on surface (Σ), this value may be discarded for the purpose of optimization because it is negative.

Let us now check the two conditions of feasibility, inequalities (76) and (78). The first one is

$$z_S\ k_A\ S_0^2 - K_S \geq 0 \tag{76}$$

Substituting numerical values gives

$$1. \times 6 \times (10.)^2 - 0.50 = + 599.5 > 0$$

The second one is

$$\frac{z_R\ K_R\ k_B}{(k_B\ \theta_{W3} - 1)^2} + \frac{z_U\ K_U\ k_C}{(k_C\ \theta_{W3} - 1)^2} - 1 > 0 \tag{78}$$

At the first stage, $\theta_1 = 0.455$. Thus, from equation (12)

$$S_1 = \frac{0.50}{0.455 \times 6 - 1} = 0.289$$

From equation (17), we have

$$U_1 = 0.20(10.0 - 0.289) = 1.942$$

From equation (59)

$$\theta_{w3} = \frac{1}{0.25}\left(1 + \frac{1.50}{1.942}\right) = 7.09$$

From equation (74)

$$\varphi(7.09) = \frac{1.50 \times 1.00 \times 1.50}{(7.09 \times 0.5 - 1)^2} + \frac{1.50 \times 1.50 \times 0.25}{(7.09 \times 0.25 - 1)^2} - 1$$

$$= 0.115 + 0.944 - 1$$

$$\varphi(7.09) = 0.059 > 0$$

The two conditions for feasibility are satisfied at operating point A.

APPENDIX III

NATURE OF THE STATIONARY POINTS OF RESPONSE SURFACE (Σ)

The first coordinate of stationary points is given by equation (71)

$$\theta_1 = \frac{1}{k_A}\left[1 \pm \sqrt{z_S\ K_S\ k_A}\right] \qquad (71)$$

Substituting numerical values for the parameters yields

$$\theta_1 = + 0.455$$

$$\theta_1 = - 0.122$$

In addition, equation (73) gives the following two values for θ_2

$$\theta_2 = + 7.18$$

$$\theta_2 = - 0.376$$

Therefore, response surface (Σ) has four stationary points given below:

A(+ 0.455, + 7.18)

B(- 0.122, + 7.18)

C(- 0.122, - 0.376)

D(+ 0.455, - 0.376)

The nature of each of these stationary points will be examined by evaluation of the Hessian matrix. As a general rule, the necessary and sufficient condition that a square matrix be positive definite is that each of the principal minors of this matrix be greater than zero. A necessary and sufficient condition for a square matrix to be negative definite is that the signs of its principal minors be alternatively negative and positive; that is the principal minor of rank r is negative if r is odd and positive if r is even. We shall now test the matrix H at the stationary points, namely A, B, C and D.

The general expression of the Hessian matrix of the objective function J is

$$H = \begin{vmatrix} \frac{1}{2} \frac{\partial^2 J}{(\partial \theta_1)^2} & \frac{1}{2} \frac{\partial^2 J}{\partial \theta_1 \partial \theta_2} \\ \frac{1}{2} \frac{\partial^2 J}{\partial \theta_1 \partial \theta_2} & \frac{1}{2} \frac{\partial^2 J}{(\partial \theta_2)^2} \end{vmatrix}$$

Let

$$h_{11} = \frac{1}{2} \frac{\partial^2 J}{(\partial \theta_1)^2}$$

$$h_{12} = \frac{1}{2} \frac{\partial^2 J}{\partial \theta_1 \partial \theta_2} = \frac{1}{2} \frac{\partial^2 J}{\partial \theta_2 \partial \theta_1}$$

$$h_{22} = \frac{1}{2} \frac{\partial^2 J}{(\partial \theta_2)^2}$$

From equation (67), we have

$$\frac{\partial J}{\partial \theta_1} = 1 - \frac{z_S \, K_S \, k_A}{(k_A \, \theta_1 - 1)^2}$$

Differentiating this again with respect to θ_1, we obtain

$$\frac{\partial^2 J}{(\partial \theta_1)^2} = \frac{2z_S\ K_S\ k_A^2}{(k_A\ \theta_1 - 1)^3}$$

Hence

$$h_{11} = \frac{z_S\ K_S\ k_A^2}{(k_A\ \theta_1 - 1)^3}$$

From equation (67), we have

$$\frac{\partial J_2}{\partial \theta_2} = 1 - \frac{z_R\ K_R\ k_B}{(k_B\ \theta_2 - 1)^2} - \frac{z_U\ K_U\ k_C}{(k_C\ \theta_2 - 1)^2}$$

Taking the derivative of this expression again with respect to θ_2 yields

$$\frac{\partial^2 J_2}{(\partial \theta_2)^2} = \frac{2\ z_R\ K_R\ k_B^2}{(k_B\ \theta_2 - 1)^3} + \frac{2\ z_U\ K_U\ k_C^2}{(k_C\ \theta_2 - 1)^3}$$

and

$$h_{22} = \frac{z_R\ K_R\ k_B^2}{(k_B\ \theta_2 - 1)^3} + \frac{z_U\ K_U\ k_C^2}{(k_C\ \theta_2 - 1)^3}$$

In addition

$$\frac{\partial^2 J_2}{\partial \theta_1 \partial \theta_2} = 0.$$

Hence

$$h_{12} = h_{21} = 0.$$

Now, the general Hessian matrix at point (θ_1, θ_2) is

$$H = \begin{vmatrix} \dfrac{z_S\, K_S\, k_A^2}{(k_A\, \theta_1 - 1)^3} & 0 \\ 0 & \dfrac{z_R\, K_R\, k_B^2}{(k_B\, \theta_2 - 1)^3} + \dfrac{z_U\, K_U\, k_C^2}{(k_C\, \theta_2 - 1)^3} \end{vmatrix} \quad (93)$$

Point A (0.455, 7.183)

Substituting the coordinates of point A in equation (93) leads to

$$H_A = \begin{vmatrix} \dfrac{1.0 \times 0.50 \times (6.)^2}{(6.00 \times 0.455 - 1)^3} & 0 \\ 0 & \dfrac{1.50 \times 1.00 \times (0.50)^2}{(0.50 \times 7.183 - 1)^3} + \dfrac{1.50 \times 1.50 \times (0.25)}{(0.25 \times 7.183 - 1)^3} \end{vmatrix}$$

$$H_A = \begin{vmatrix} \dfrac{18}{(1.73)^3} & 0 \\ 0 & \dfrac{0.375}{(2.59)^3} + \dfrac{0.140}{(0.796)^3} \end{vmatrix}$$

Finally

$$H_A = \begin{vmatrix} +3.48 & 0 \\ 0 & +0.299 \end{vmatrix}$$

H_A is positive definite. The two principal minors are $+3.48 > 0$ and $(+3.48)(+0.299) - 0 > 0$. Hence point A(+ 0.455, + 7.183) is a minimum on response surface (Σ). The procedure set up in Section IV.5 to generate the contours around this point has been implemented by means of subroutine ISOBAT (see Figure 20).

Point B (- 0.122, + 7.18)

Substituting θ_1 = - 0.122 and θ_2 = + 7.18 in to equation (88) yields

$$H_B = \begin{vmatrix} \dfrac{18}{(-1.732)^3} & 0 \\ 0 & \dfrac{0.375}{(2.59)^3} + \dfrac{0.140}{(0.796)^3} \end{vmatrix}$$

$$H_B = \begin{vmatrix} -3.46 & 0 \\ 0 & +0.299 \end{vmatrix}$$

H_B is not positive nor negative definite because its principal minors are $-3.46 < 0$ and $(-3.46)(+0.299) < 0$. As a result, point B(- 0.122, + 7.18) is a saddle point on response surface (Σ).

Point C (- 0.122, - 0.376)

This point has the abscissa of B and the ordinate θ_2 = - 0.376. Thus

$$h_{11} = -3.46$$

and

$$h_{22} = \frac{0.375}{[0.50 \times (-0.376) - 1]^3} + \frac{0.140}{[0.25 \times (-0.376) - 1]^3}$$

$$= \frac{0.375}{(-1.188)^3} + \frac{0.140}{(-1.094)^3}$$

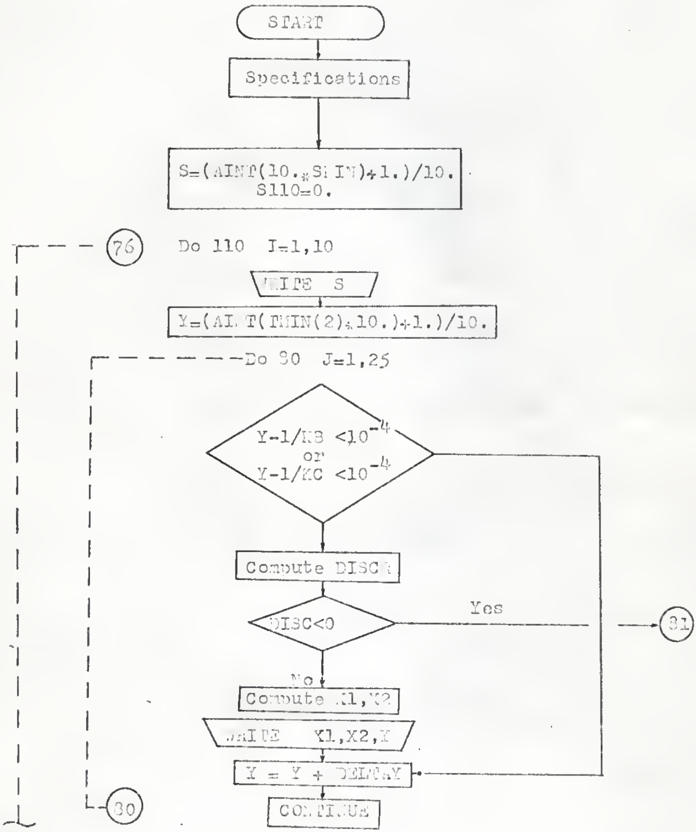

Figure 20(a). Flow - chart of subroutine ISOBAT

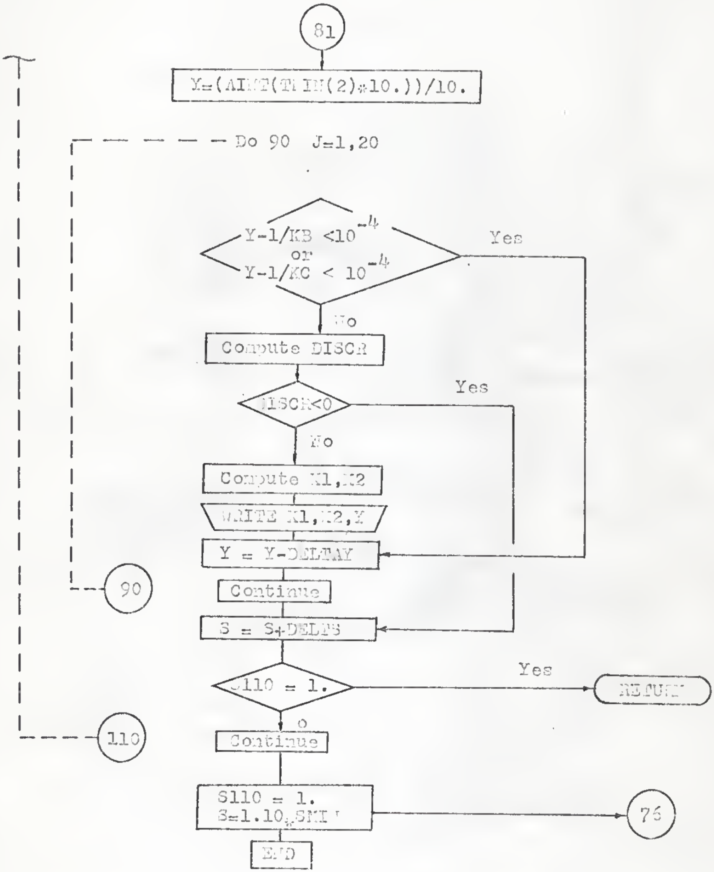

Figure 20(b). End of flow - chart of subroutine ISOBAT

$$= -0.331$$

The Hessian matrix at point C is

$$H_C = \begin{vmatrix} -3.46 & 0 \\ 0 & -0.331 \end{vmatrix}$$

H_C is negative definite because its principal minors are $-3.46 < 0$ and $(-3.46)(-0.331) > 0$. Therefore, point C (-0.122, -0.376) is a maximum on (Σ).

<u>Point D (+0.455, -0.376)</u>

This point has the same abscissa as A and the same ordinate as C. Matrix H_D can immediately be written as

$$H_D = \begin{vmatrix} +3.48 & 0 \\ 0 & -0.331 \end{vmatrix}$$

H_D is neither positive definite nor negative definite because its principal minors are $+3.48 > 0$ and $(+3.48)(-0.331) < 0$. Therefore, point D is a saddle point on response surface (Σ).

APPENDIX IV

COMPUTATIONAL SCHEME FOR THE SEARCH TECHNIQUE APPROACH

Basic features of the sequential Simplex technique (11).

We consider, initially, the minimization of a function of n variables, without constraints. P_0, P_1, ..., P_n are the (n+1) points of the current simplex in n-dimensional space. We write y_i for the function value at P_i and define h as the suffix such that

$$y_h = \max_i(y_i)$$

and ℓ as the suffix such that

$$y_\ell = \min_i (y_i)$$

Further we define $\overline{P}$ as the centroid of the points with $i \neq h$, and write $[P_i \; P_j]$ for the distance from P_i to P_j. At each stage in the process P_h is replaced by a new point; three operations are used - REFLECTION, CONTRACTION, and EXPANSION. These are defined as follows: The reflection of P_h is denoted by P*, and its co-ordinates are defined by the relation

$$P^* = (1 + \alpha)\overline{P} - \alpha P_h$$

where α is a positive constant, the reflection coefficient. Thus P* is on the line joining P_h and $\overline{P}$, on the far side of $\overline{P}$ from P_h with $[P^* \; \overline{P}] = \alpha[P_h \; \overline{P}]$. If y* lies between y_h and y_ℓ, then P_h is replaced by P^* and we start again with the new simplex.

If $y^* < y_\ell$, i.e., if reflection has produced a new minimum, then we expand P^* to P^{**} by the relation

$$P^{**} = \gamma P^* + (1 - \gamma)\overline{P}$$

The expansion coefficient γ, which is greater than unity, is the ratio of the distance $[P^{**}\ \overline{P}]$ to $[P^*\ \overline{P}]$. If $y^{**} \leq y$ we replace P_h by P^{**} and restart the process; but if $y^{**} > y_\ell$ then we have failed to find a better point by expansion, and we replace P_h by P^* before restarting.

If on reflecting P to P^* we find that $y^* > y_i$ for all $i \neq h$, i.e. that replacing P_h by P^* leaves y^* the maximum, then we define a new P_h to be either the old P_h or P^*, whichever has the lower y value, and form

$$P^{**} = \beta P_h + (1 - \beta)\overline{P}.$$

The contraction coefficient β lies between 0 and 1 and is the ratio of the distance $[P^{**}\ \overline{P}]$ to $[P_h\ \overline{P}]$. We then accept P^{**} for P_h and restart, unless $y^{**} > \min(y_h, y^*)$, i.e., the contracted point is worse than the better of P_h and P^*. For such a failed contraction we replace all the P_i's by $(P_i + P_\ell)/2$ and restart the process.

The criterion adopted to stop the search is to compare the "standard error" of the y's in the form $\sqrt{\Sigma(y_i - \overline{y})^2/n}$ with a pre-set value.

The name SIMPLE has been given to the corresponding FORTRAN subroutine for this search procedure.

In order to perform a search the value of the objective function should be available for a given decision vector. The FORTRAN name of this subroutine is OBJ. Flow-chart of subroutine SIMPLE appears in Figure 21.

Constraints on the volume to be searched.

If, for example, one of the x_i must be non-negative in a minimization problem, then the original sequential simplex search method may be adopted as follows: The scale of the x concerned can be transformed, e.g., the function can be modified to take a large positive value for all negative x. In the latter case any trespassing by the simplex over the border will be followed automatically by contraction moves which will eventually keep it inside. This method is illustrated in Figure 22. If the reflected point P* trespasses the border line of the permitted region, a contraction follows, which results in the new simplex P_1, P_2, P**. If the expanded point P** trespasses the border line, P** is replaced by the reflected point P* which was within the permitted region. In either case the new simplex is within the constraint and the iteration process can be carried on.

Determination of the optimal policy by the empirical search.

The various components of the optimization problem have been stated in Section IV. The procedure consists of the following steps:

Step 1

Compute $\theta_{1\ opt}$ by equation (72) and check the first condition, equation (76).

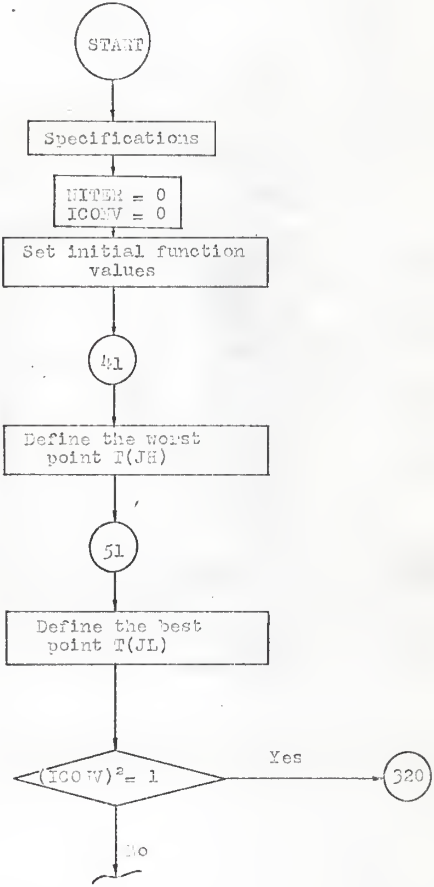

Figure 21(a). Flow - chart of subroutine SIMPLE

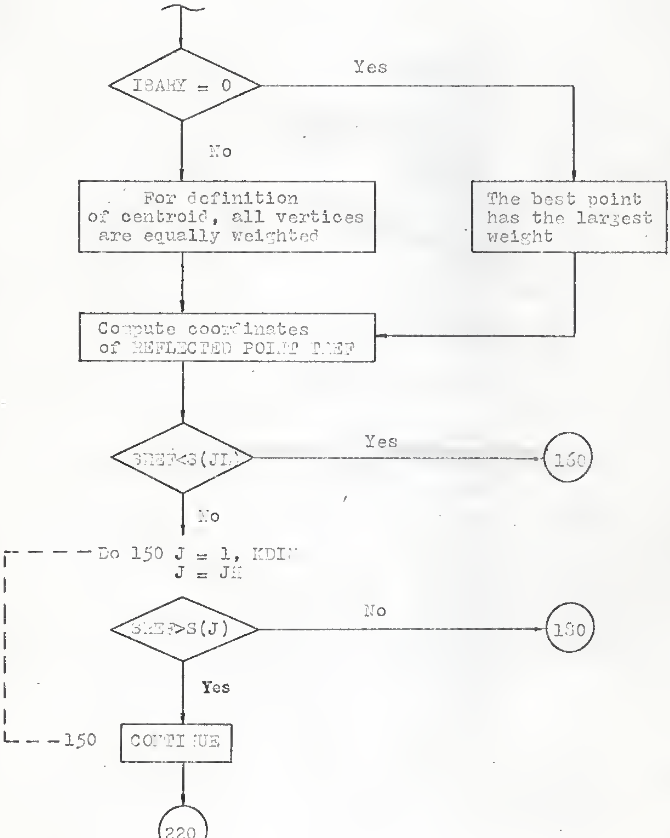

Figure 21(b). Continuation

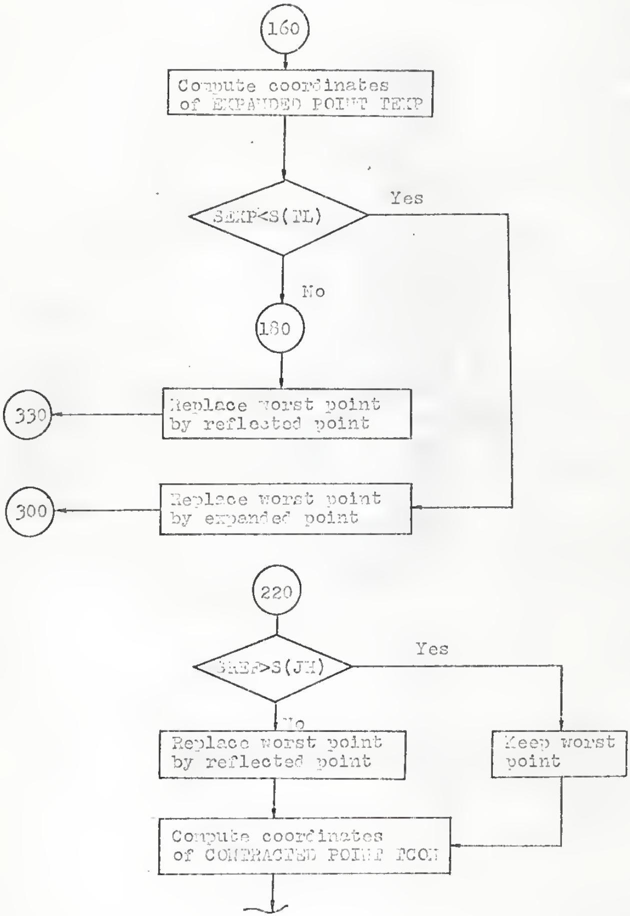

Figure 21(c). Continuation

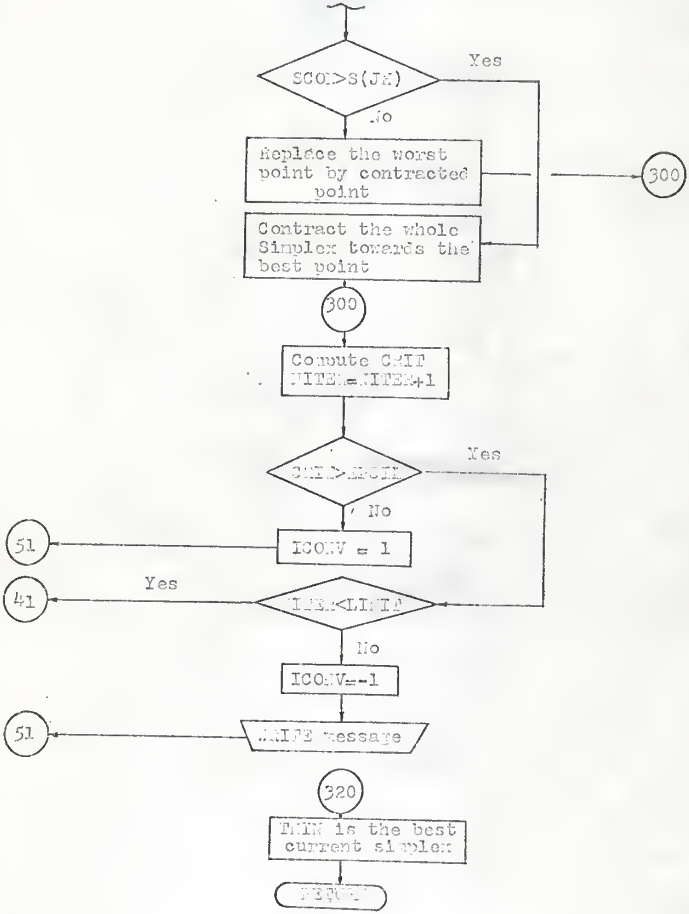

Figure 21(d). End of subroutine SIMPLE

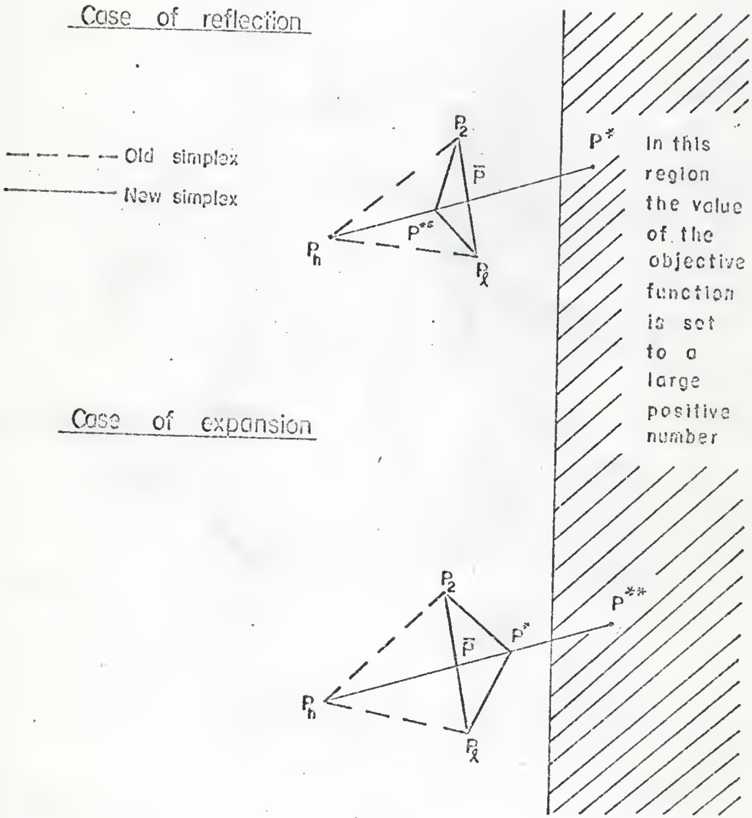

Fig. 22. Treatment of inequality constraints on the independent variables in simplex technique.

Step 2

Determine $\theta_{2\ opt}$ by solving equation (73). Compute θ_{w2} and check the second condition, equation (78).

Step 3

Initialize counters and set the first guess for optimal solution.

Step 4

In order to perform the search an initial simplex and the inequality constraints should be specified. Thus this step consists of setting the initial simplex in the neighborhood of the optimal point already defined in Steps 1 and 2 and computing θ_{w3} corresponding to the initial guess for θ_2 set in Step 3.

Step 5

Call the search technique. If the resulting point is close enough to the initial guess, its coordinates constitute the optimal policy. If not, the result of the search serves as starting point for the next iteration.

Step 6

After convergence the corresponding state variables can be computed using the performance equations.

APPENDIX V

DESCRIPTION OF MAIN PROGRAM MICU20

The main program for solving this problem has been given the name MICU20. In this paragraph all FORTRAN locations will be written with capital characters.

The program MICU20 consists of six parts as illustrated in Figure 23.

First part:

It contains the speciffications, the definition of statement functions needed in the remainder of the program, the input statements for the physical and economical parameters and the input statements of option parameters NOPT, ICURV and ICONT and the search parameters. In addition, it performs the echo-check of these data.

Second part:

It is devoted to the determination of the optimal policy. Note that equation (73) which is of degree 4, has been solved by the NEWTON method. The name of the subroutine which performs this search is precisely NEWTON.

The values of the first members of inequalities given by equations (76) and (78) are called respectively TEST1 and TEST2.

Third part:

This part deals with the case where the operating policy (θ_1, θ_2) is fixed by user without being optimal.

It simply consists of reading the chosen decision variables, and calling subroutine OBJ which gives the value of the objective function.

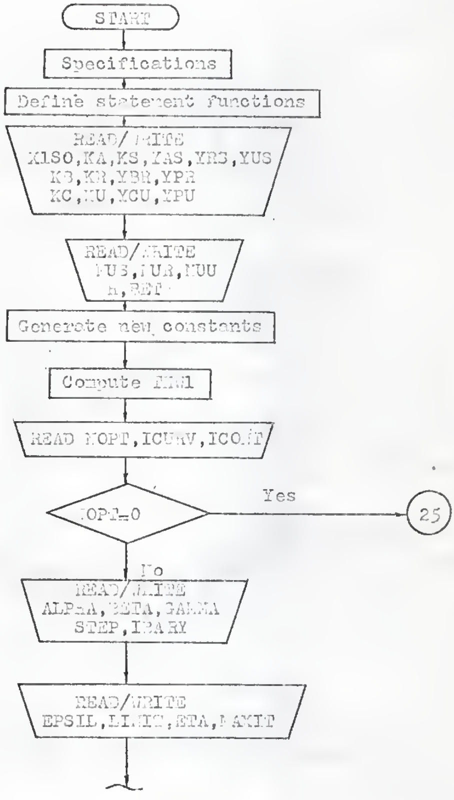

Figure 23(a). Flow-chart of main program MICU20
First part: Specifications, statement functions
& data echo check

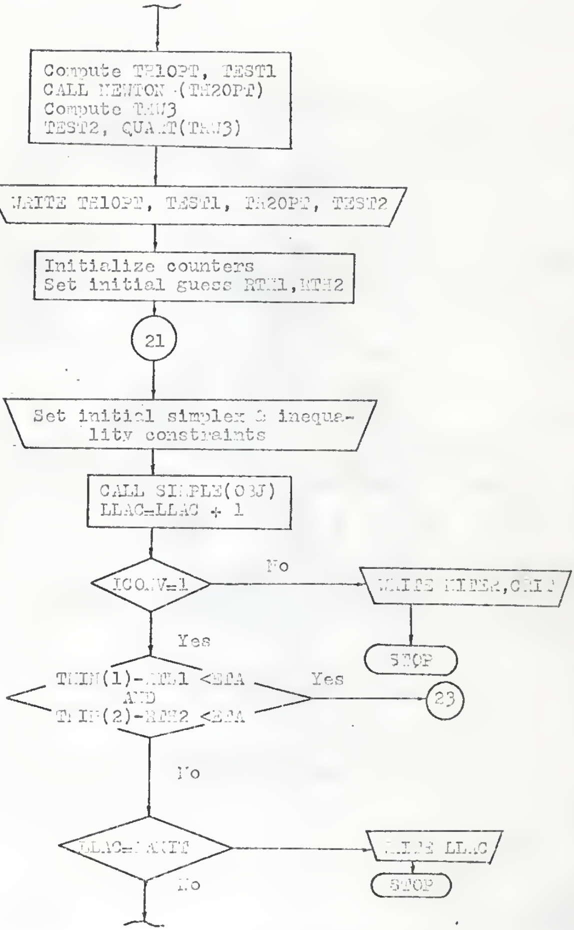

Figure 23(b). Second part: Determination of optimal policy

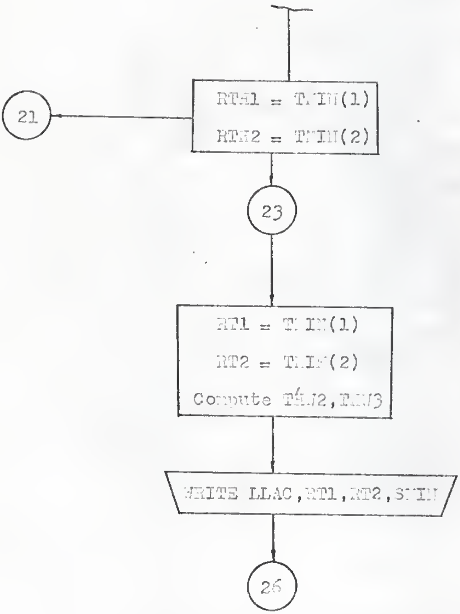

Figure 23(c). End of second part

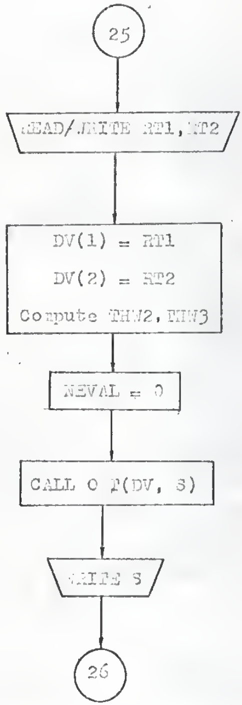

Figure 23(d). Third part: Case of non-optimal policy

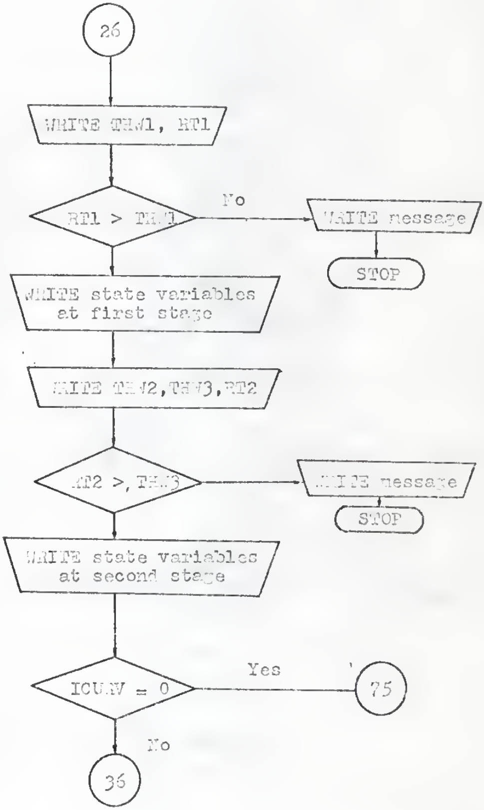

Figure 23(e). Fourth part: State variables of optimal policy

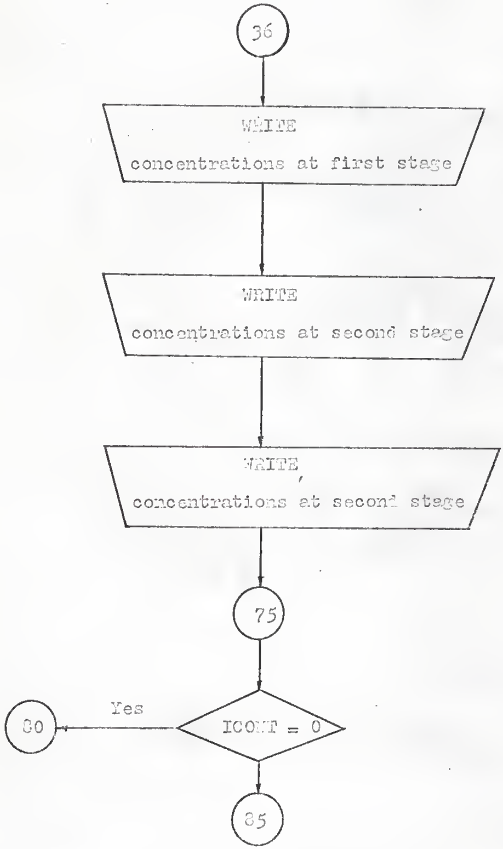

Figure 23(f). Fifth part: Concentration curves

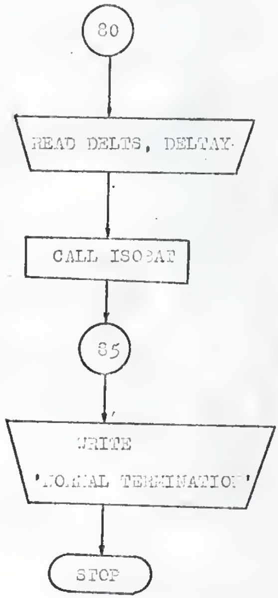

Figure 23(g). Part VI: Drawing of contours

End of program MICU20

Fourth part:

The state variables resulting from the previously chosen policy are determined.

Fifth part:

In this part the concentration curves are plotted. In addition the slopes at the points of discontinuity are determined, according to Appendix I.

Sixth part:

By calling subroutine ISOBAT various contours around the optimal point are generated using the procedure described in section IV.5. The meaning of the symbols in Figure 23 appears in Table 2. Table 3 contains the list of the required data cards.

TABLE 2

MAIN FORTRAN SYMBOLS

Symbol	Meaning or corresponding algebraic variable
MICU20	Main routine
SIMPLE	Subroutine for SIMPLEX search technique
NEWTON	Subroutine implementing NEWTON'S method for root searching
ISOBAT	Subroutine to generate the contours around the optimal point on the response surface
OBJ	Subroutine for computing objective function
QUART	Function $\varphi(\theta_2)$
KA, KB, KC	k_A, k_B, k_C
KS, KR, KU	K_S, K_R, K_U
MUS, MUR, MUU	z_S, z_R, z_U
THW1, THW2, THW3	θ_{w1}, θ_{w2}, θ_{w3}
DELTAS, DELTAY	Increment on objective function and θ_2 respectively for contours drawing
NDIM	Dimensionality of search
ALPHA, BETA, GAMMA	α, β, γ
IBARY	Option parameter for SIMPLE
EPSIL	Convergence criterion for SIMPLE
LIMIT	Maximum number of iterations to be performed during the search
ICONV	Convergence index
TMIN	Optimal decision vector
NITER	Number of iterations actually performed in SIMPLE
NEVAL	Number of function evaluations

TABLE 2 (Cont.)

X1S1, X2A1, X1R1, X1U1	S_1, A, R_1, U_1
DELTAS	$S_0 - S_1$
DELTAR	$R_1 - R_2$
DELTAU	$U_1 - U_2$
X1R2, X1U2, X2B2, X2C2, X1P2	R_2, U_2, B, C, P
R, BET	Recycle ratio and clarifyer efficiency
W2, W3	θ_{w2}, θ_{w3}
NOPT, 1CURV, 1CONT	Option parameters
ETA	Criterion for over-all convergence
MAXIT	Maximum number of iterations for optimization loop
TEST1	Value of first member of inequality (76)
TEST2	Value of first member of inequality (78)
TH1OPT, TH2OPT	θ_{1opt}, θ_{2opt}
LLAC	Iterations counter
TH	Current Simplex
RT1, RT2	Operating residence times
S	Objective function
DX1S1	$\left.\frac{dS_1}{d\theta_1}\right\vert_{\theta_{w1}}$
DX2A1	$\left.\frac{dA}{d\theta_1}\right\vert_{\theta_{w1}}$
DX1R1, DX1U1	$\left.\frac{dR_1}{d\theta_1}\right\vert_{\theta_{w1}}$, $\left.\frac{dU_1}{d\theta_1}\right\vert_{\theta_{w1}}$

TABLE 2 (Cont.)

T	Current decision vector in SIMPLE
SH	Highest function value (y_h)
SL	Lowest function value (y_ℓ)
TBAR	Coordinates of the centroid
SBAR	Value of the objective function at centroid
TREF, SREF	Coordinates and function value at reflected point
TEXP, SEXP	Coordinates and function value at expanded point

TABLE 3

DATA CARDS

Card	
1 and 2	Title
3	X1S0, KA, KS, YAS, YRS, YUS
4	KB, KR, YBR, YPR
5	KC, KU, YCU, YPU
6	MUS, MUR, MUU
7	NOPT, ICURV, ICONT
8	R, BET * If NOPT = 0 and ICONT = 0
9	RT1, RT2 * If NOPT ≠ 0 and ICONT = 0
10	ALPHA, BETA, GAMMA, STEP, IBARY
11	EPSIL, LIMIT, ETA, MAXIT * If NOPT ≠ 0 and ICONT ≠ 0
12	DELTS, DELTAY

SIMULATION AND OPTIMIZATION OF A TWO STAGE CONTINUOUS ANAEROBIC DIGESTER SYSTEM

by

Jean-Claude Baltes

Engineer, Ensic, France 1963

AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1969

ABSTRACT

This work considers an anaerobic digestion process represented by a two-step mechanism and carried out in a two-stage continuous digester system. A mathematical formulation of the kinetic and flow models has been given, which allows simulation of the system. On this basis, an objective function of economic type can be constructed, the minimization of which yields the optimal design. The analysis of the system by means of this mathematical formulation also shows that wash-out times are important design parameters. Finally, a contact process in which organisms are recycled to the second stage is compared to the conventional process. From this comparison it can be concluded that the contact process has definite advantages over the conventional process.