$\overline{W}$ = average dimensionless axial velocity
x, y, z = orthogonal Cartesian coordinates
X, Y, Z = dimensionless coordinates
$\partial p/\partial z$ = hydrostatic axial pressure gradient
μ = dynamic viscosity of blood, [the viscosity may be taken as a constant at shear rates exceeding 50 to 100 sec.$^{-1}$. At lesser shear rates, blood is non-Newtonian and is adequately described by the Casson equation (*13*)]
ν = kinematic viscosity of blood
ρ = density of blood
$(\ )_\infty$ = condition at $Y = 0$
$(\ )_0$ = condition at $Z = 0$

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Optimal Operation of a Variable-Volume Stirred Tank Reactor

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For certain classes of chemical reactions, it is possible to increase the yield of the desired products by choosing appropriate variable-volume operating policies. An analysis of the steady state and semibatch operation of a stirred tank reactor demonstrates operating policies for both the isothermal and adiabatic case to maximize the steady state yield and to produce an improved semibatch yield. Computations carried out by using an analogue computer with a digital logic expansion system demonstrate further relationships between yield increase and operating policy.

The continuous stirred tank or backmixed reactor is a very common chemical engineering processing unit. A considerable amount of analysis regarding the design, operation, and control of these units has produced much useful information for engineers (*1, 9*). Generally, these reactors are operated at or near steady state, with the mean residence time adjusted to produce the optimum or desired product yield. It has been observed (*7*) that in selected cases the value of an increased yield which might be obtainable from a periodic operating policy would be enough to offset the additional costs resulting from increased handling and storage. In order to investigate the economic feasibility of such schemes, it is necessary to quantitatively investigate the relationships between the yield of a backmixed reactor and the operating variables encountered during variable-volume operation. The concept of increasing the yield of a chemical reactor by various types of periodic operation is becoming of interest to chemical engineers (*3* to *8*). However, the variable-volume periodic reactor has been neglected, although the concept of a variable-volume periodic reactor abounds in nature, perhaps the foremost example being the human lung.

In this work, analysis is carried out on isothermal and adiabatic stirred tank reactors. These two extreme or limiting cases represent a logical starting point but by no means cover the entire range of operating conditions found in practice. Although it appears that the possible obtainable improved yield for a periodic operation will be more dramatic for higher order reactions, this study concentrates on the irreversible first-order reaction. The techniques of analysis are easily extendable to higher-order reactions. This approach is justified on two counts, the one being that a very large class of reactions may be treated at least as pseudo first-order reactions, and the other being the simplicity of the case which hopefully results in increased insight into the overall situation of variable-volume operation.

While the isothermal case is almost completely amenable to analytical solution, the adiabatic case requires the use of an analogue computer with an associated digital logic expansion system to solve the working equations and to provide some insight into the factors influencing the relationships between yield increase and operating policy.

The following general equations may be written for a completely backmixed stirred tank reactor as depicted in Figure 1, assuming negligible volume change due to chemical reaction, but not necessarily operating at constant volume.

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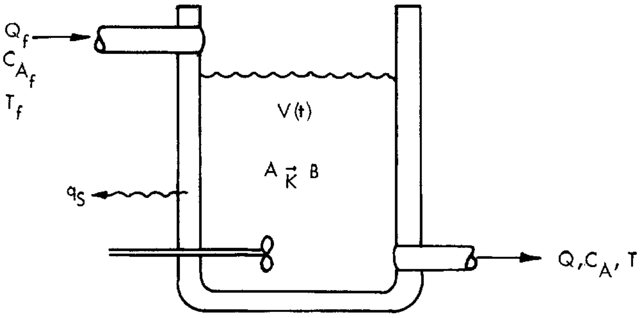

Fig. 1. Nomenclature.

Material balance (*A* disappearing)

$$\frac{d}{dt}(VC_A) = Q_f C_{Af} - QC_A - R_A \qquad (1)$$

For the irreversible first-order reaction $R_A = KVC_A$

Energy balance

$$\frac{d}{dt}(VT) = Q_f T_f - QT + \frac{(-\Delta H)KC_A V}{\rho C_p} - \frac{q_s V}{\rho C_p} \qquad (2)$$

Flow-volume

$$\frac{dV}{dt} = Q_f - Q \qquad (3)$$

For small temperature changes, K may be expressed as

$$K = K_0 + b(T - T_0) \qquad (4)$$

where b will be a positive constant for any reaction.

It is convenient to put all of these relations into dimensionless form by introducing the following variables:

$$K^* = K/K_0 \qquad (a)$$

$$T^* = T/T_f \qquad (b)$$

$$T_0^* = T_0/T_f \qquad (c)$$

$$C^* = C_A/C_{AF} \qquad (d)$$

$$t^* = tQ_R/V_R \qquad (e)$$

$$t^* = t/\tau \qquad (f) \quad (5)$$

$$Q^* = Q/Q_R \qquad (a)$$

$$Q_f^* = Q_f/Q_R \qquad (b)$$

$$V^* = V/V_R \qquad (c) \quad (6)$$

The reference flow rate for the constant volume case is simply $Q_R = Q_f = Q$, while the reference volume is simply $V_R = V = V_{\max}$. τ for this case represents the true mean residence time. T_f, C_{Af}, V_R, and Q_R are regarded as constants. For variable-volume operation, Q_R and V_R must be selected carefully, and the resulting τ may be referred to as a pseudo residence time.

The following dimensionless parameters are also conveniently formed.

Relative energy parameter

$$R = \frac{(-\Delta H)C_{Af}}{\rho C_p T_f} \qquad (a)$$

Relative rate parameter

$$L = bT_f/K_0 \qquad (b)$$

Relative time parameter

$$P = K_0 V_R/Q_R \qquad (c)$$

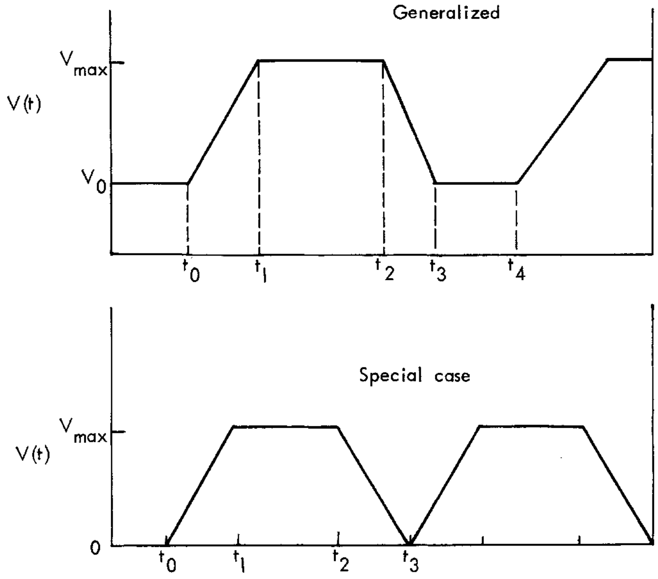

Fig. 2. Schema—semibatch operation nomenclature: A. generalized, B. special case.

Relative heat parameter

$$H = q_s V_R/\rho C_p T_f Q_R \qquad (d) \quad (7)$$

The parameter R is simply the relative adiabatic temperature rise, which is the ratio of the temperature rise corresponding to complete conversion, and the feed temperature T_f. The parameter P may be considered the ratio of a reaction velocity K_0 to the space velocity Q_R/V_R. The parameters L and H have no particular physical significance and are merely convenient collections of constants. The dimensionless equations for a constant volume reactor are, then

$$\frac{dC^*}{dt^*} = 1 - (1 + PK^*)C^* \qquad (8)$$

$$\frac{dT^*}{dt^*} = 1 - T^* + K^*C^*PR - H \qquad (9)$$

$$K^* = 1 + L(T^* - T_0^*) \qquad (10)$$

and for a variable-volume reactor

$$\frac{dC^*}{dt^*} = \frac{Q_f^*}{V^*}(1 - C^*) - PK^*C^* \qquad (11)$$

$$\frac{dT^*}{dt^*} = \frac{Q_f^*}{V^*}(1 - T^*) + RPK^*C^* - H \qquad (12)$$

$$V^* = V_0^* + \int_0^{t^*} (Q_f^* - Q^*)dt^* \qquad (13)$$

The dimensionless equations are nonlinear, owing to the appearance of the product of the rate constant and concentration, and are also coupled in temperature and concentration. The dimensionless equations for the variable-volume reactor may also have variable coefficients. Fortunately, for several cases the solutions are straightforward.

ISOTHERMAL OPERATION

For isothermal operation, with $K = K_0$, only the concentration equation is needed:

$$\frac{dC^*}{dt^*} = \frac{Q_f^*}{V^*}(1 - C^*) - PC^* \qquad (14)$$

Constant Volume Operation (CST)

The solutions for this trivial case may be written directly, since $Q_f^* = V^* = 1.0$.

Steady state solution

$$C^* = \frac{1}{1+P} \qquad (15)$$

The steady state yield may be defined as

$$\eta_{CST} = 1 - C^* = P/(1+P) \qquad (16)$$

The maximum yield $\eta = 1$, of course, occurs when $P = \infty$, which corresponds to a batch reactor with no flow.

Transient solution

$$C^* = \frac{1}{1+P} + \left[C_0^* - \frac{1}{1+P}\right] e^{-(1+P)t^*} \qquad (17)$$

Variable Volume Operation (VVO)

The solutions for the two trivial variable-volume cases of the reactor filling ($Q = 0$) or emptying ($Q_f = 0$) may also be written directly:

$Q = 0, Q_R = Q_f, V_R = V_0$

$$C^* = \frac{1}{P(1+t^*)}[1 + (PC_0^* - 1)\, e^{-Pt^*}] \qquad (18)$$

$Q_f = 0$

$$C^* = C_0^*\, e^{-Pt^*} \qquad (19)$$

For the general case where $Q \neq Q_f$, it is necessary to carefully define Q_R and V_R as follows:

$$\begin{array}{llll} Q_f < Q & Q_R = Q - Q_f & V_R = V_0 & \tau = V_0/Q_R \\ Q_f > Q & Q_R = Q_f - Q & V_R = V_0 & \tau = V_0/Q_R \end{array} \qquad (20)$$

In general, Equation (14) cannot be integrated directly, except for the many cases where

$$\frac{Q}{|Q - Q_f|} = Q^* = \text{an integer, } m$$

$Q_f > Q$

For example, if $Q_f = 2Q$, $Q^* = 1$, and

$$C^* = \frac{2[P(1+t^*) - 1] + [C_0^*P^2 - 2(P-1)]e^{-Pt^*}}{P^2(1+t^*)^2} \qquad (21)$$

The general solution for this case is

$$C^* = \frac{(m+1)(A_1) + e^{-Pt^*}[C_0^*P^{m+1} - (m+1)(A_2)]}{P^{m+1}(1+t^*)^{m+1}} \qquad (22)$$

where

$$A_1 = P^m(1+t^*)^m - mP^{m-1}(1+t^*)^{m-1} + m(m-1)P^{m-2}(1+t^*)^{m-2} + \ldots (-1)^m m!$$

$$A_2 = P^m - mP^{m-1} + m(m-1)P^{m-2} + \ldots$$

$Q_f < Q$

For example, $Q = 2Q_f$, $Q^* = 2$

$$C^* = 1 - P(1-t^*)e^{P(1-t^*)} \left(\sum_{n=0}^{\infty} \left\{ \frac{(-1)^n P^n[1 - (1-t^*)^n]}{n \cdot n!} \right\} - \ln(1-t^*) \right) + (1-t^*)(C_0^* - 1)e^{-Pt^*} \qquad (23)$$

and the general solution is

$$C^* = \frac{1}{(m-2)!} \sum_{j=0}^{m-2} \left\{ (-1)^j (m-2-j)! P^j [(1-t^*)^j - e^{-Pt^*}(1-t^*)^{m-1}] \right\} + \frac{(-1)^{m-1}[P(1-t^*)]^{m-1} e^{P(1-t^*)}}{(m-2)!}[B_1] + C_0^*(1-t^*)^{m-1} e^{-Pt^*} \qquad (24)$$

where

$$B_1 = \sum_{n=1}^{\infty} \left\{ \frac{(-1)^n P^n [1 - (1-t^*)^n]}{n \cdot n!} \right\} - \ln(1-t^*)$$

Many variable-volume operating policies can now be evaluated by using these relations as approximations.

Semibatch Operation (SBO)

In order to demonstrate the yield increase obtainable by variable-volume operation and to determine the parameters which affect yield increase, an operation which is amenable to computation by using the above relations is chosen. In this operation, the reactor volume is alternated between a minimum and a maximum by adjusting the input and output flow rates. After a few cycles, the reactor reaches a pseudo steady state; that is, the concentration and volume profiles repeat in each cycle identically.

The generalized semibatch operation may be described as follows:

$$\begin{array}{llll} t = t_0 & Q_f = 0 & Q = 0 & V = V_0 \\ t_0 \leq t \leq t_1 & Q_f = Q_{fSBO} & Q = 0 & V = V_0 + Q_f(t - t_0) \\ t_1 \leq t \leq t_2 & Q_f = 0 & Q = 0 & V = V_{\max} \\ t_2 \leq t \leq t_3 & Q_f = 0 & Q = Q & V = V_{\max} - Q(t - t_2) \\ t_3 \leq t \leq t_4 & Q_f = 0 & Q = 0 & V = V_0 \end{array} \qquad (25)$$

This repeating cycle is depicted in Figure 2A.

The yield for this generalized semibatch operation (SBO) may be best evaluated by defining an equivalent Q_{CST}, by setting $V_R = V_{\max}$, $Q_R = Q_{CST}$, and by computing the yield relative to that of an equivalent CST operation, where

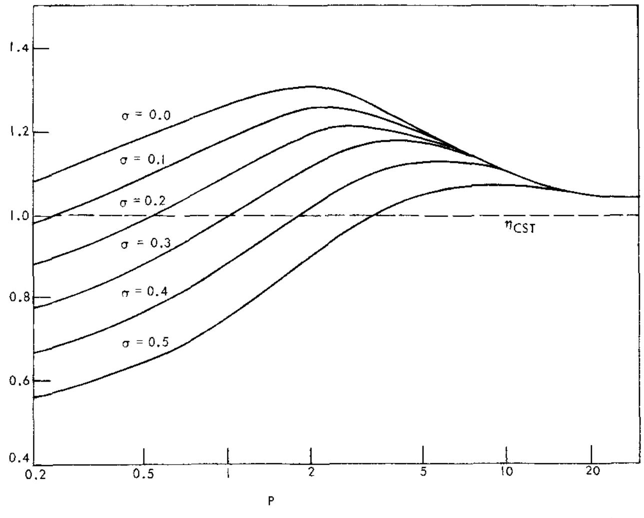

Fig. 3. Effect of relative time parameters on relative yield for isothermal SBO.

$$Q_{CST} = Q_{fSBO}\left(\frac{t_1 - t_0}{t_4 - t_0}\right) \qquad (26)$$

$$\eta \equiv \frac{\eta_{SBO}}{\eta_{CST}} = \left(1 + \frac{1}{P}\right)\left\{1 - \left(\frac{e^{P_1} - 1}{P_1}\right)\left(\frac{e^{-P_2} - e^{-P_3}}{P_3 - P_2}\right)\left[\frac{P_4}{P - (P - P_4)e^{-P_4}}\right]\right\} \qquad (27)$$

$$\eta_{SBO} = \frac{\int_{t_0}^{t_1} Q_f C_f dt - \int_{t_2}^{t_3} Q C_A dt}{\int_{t_0}^{t_1} Q_f C_f dt} \qquad (28)$$

$$P = \frac{KV_{\max}}{Q_{CST}} \text{ and } P_i = Kt_i \qquad (29)$$

To clearly demonstrate the yield increase obtainable, the special case where $V_0 = 0$ and no down time ($t_4 - t_3 = 0$) is examined, with equal filling and emptying times. With $t_0 = 0$, and $Q_{CST} = Q_{fSBO}\ (t_1/t_3)$, where the fraction filling time σ is expressed as

$$\sigma = t_1/t_3$$

then

$$\eta = \frac{\eta_{SBO}}{\eta_{CST}} = \left(1 + \frac{1}{P}\right)\left[1 - \frac{(e^{\sigma P} - 1)^2}{(\sigma P)^2} e^{-P}\right] \qquad (30)$$

Figure 3 shows this quantity as a function of the fractional filling time and the relative time parameter P. The maximum obtainable yield occurs at a $P = 1.8$ and is 29.8% greater than the corresponding CST yield. Since this occurs at a filling time of zero, this case corresponds to the limiting situation of a batch reactor (or of a plug flow reactor with the same residence time). The yield for either of these limiting cases may be written as

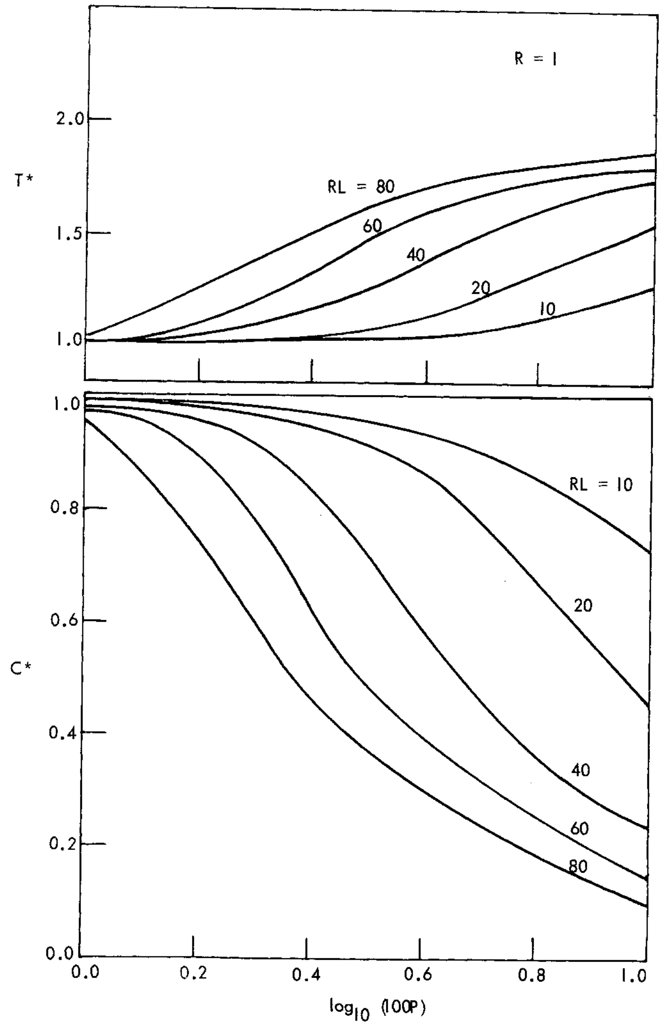

Fig. 4. CST adiabatic results.

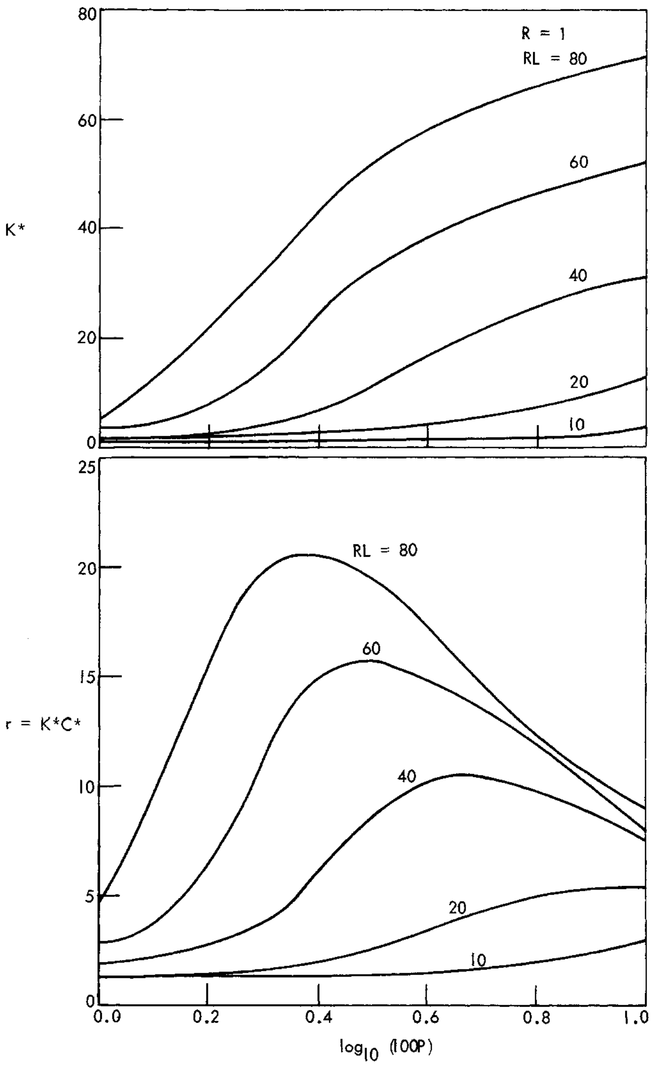

Fig. 5. CST adiabatic results.

$$\eta_{PFR} = 1 - e^{-P} \qquad (31)$$

In other words, the maximum relative yield is then

$$\eta_{\max} = \frac{\eta_{SBO}}{\eta_{CST}} = \frac{\eta_{PFR}}{\eta_{CST}} = \frac{1 - e^{-P}}{P/(1 + P)} \qquad (32)$$

This may be solved directly for the value of P which maximizes η by

$$e^{-P}[1 + P + P^2] = 1$$

from which is obtained

$$P = 1.8 \quad \eta = 1.30 \quad C^*_{CST} = 0.356 \quad C^*_{PFR} = 0.166$$

ADIABATIC OPERATION

Constant Volume Operation (CST)

The description of the adiabatic operation of a backmixed reactor requires that the energy balance and rate equations be solved simultaneously with the concentration equation, subject to the volume policy imposed, and therefore represents a much more difficult mathematical problem. It is again instructive to examine the constant volume

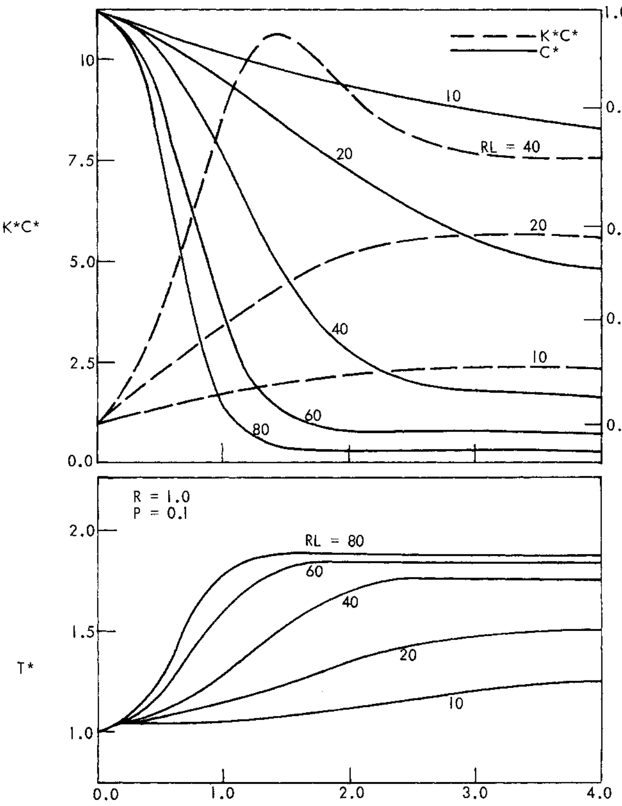

Fig. 6. Effect of RL on transient adiabatic CST behavior.

(CST) case first and demonstrate the optimal policy for that limiting case.

The basic relations for steady state operation become

$$C^* = 1 - PK^*C^* \quad P = KV_{\max}/Q_{\text{CST}} \tag{33}$$

$$T^* = 1 + RPK^*C^* \tag{34}$$

$$K^* = 1 + L(T^* - 1) \quad (T_0 = T_f) \tag{35}$$

These may be solved simultaneously to give

$$C^* = \frac{(S + P + 1) - \sqrt{(S + P + 1)^2 - 4S}}{2S} \tag{36}$$

$$K^* = \frac{1}{P}\left[\frac{2S}{(S + P + 1) - \sqrt{(S + P + 1)^2 - 4S}} - 1\right] \tag{37}$$

$$T^* = 1 + R - \frac{1}{2LP}[(S + P + 1) - \sqrt{(S + P + 1)^2 - 4S}] \tag{38}$$

$$S = RLP$$

If the dimensionless reaction rate K^*C^* is denoted by r, the equation relating the rate of consumption of A to r is

$$\text{Consumption rate of } A = Q_f(C_{Af} - C_A) = V_{\max}K_fC_{Af}r \tag{39}$$

It is apparent that $r = r(RL, P)$. For a given RL, differential calculus may be used to determine the value of P which maximizes r and hence determines the optimum residence time. Given P at $r_{\max}$, the value of $r_{\max}$ and the corresponding values of C^*, K^*, and T^* may be obtained in terms of RL. The results are

$$r_{\max} = \frac{(RL + 1)^2}{4RL} \tag{40}$$

$$P_{rm} = \frac{2(RL - 1)}{(RL + 1)^2} \tag{41}$$

$$C^*_{rm} = \frac{1}{2} + \frac{1}{2RL} \tag{42}$$

$$T^*_{rm} = 1 + \frac{R}{2} - \frac{1}{2L} \tag{43}$$

$$K^*_{rm} = \frac{(RL + 1)}{2} \tag{44}$$

Note that R and L usually occur in combination and uniquely determine the optimal policy for the CST adiabatic case. For example, if $RL >> 1$, the maximum consumption of A occurs at the residence time which produces $C^* = 0.5$, that is, 50% conversion. Of course, if an Arrhenius expression for the reaction velocity were used, different expressions would be obtained for the above variables at the maximum reaction rate. At low values of RL, that is, reactions which are only slightly exothermic or which have a small temperature dependency, the above expressions closely approximate the values obtained by using the Arrhenius expression for reaction velocity.

Figures 4 and 5 show C^*, T^*, K^*, and r as functions of R, L, P, and RL. These results were obtained by using an EAI Tr-48 analogue computer and by generating P instead of time as the independent variable. (Actually, log P was generated, since P ranges over several orders of magnitude in the regions of interest.)

The transient solutions of the adiabatic CST equations [Equations (8), (9), (10), with $H = 0$] were also determined by using the analogue computer, since analytical

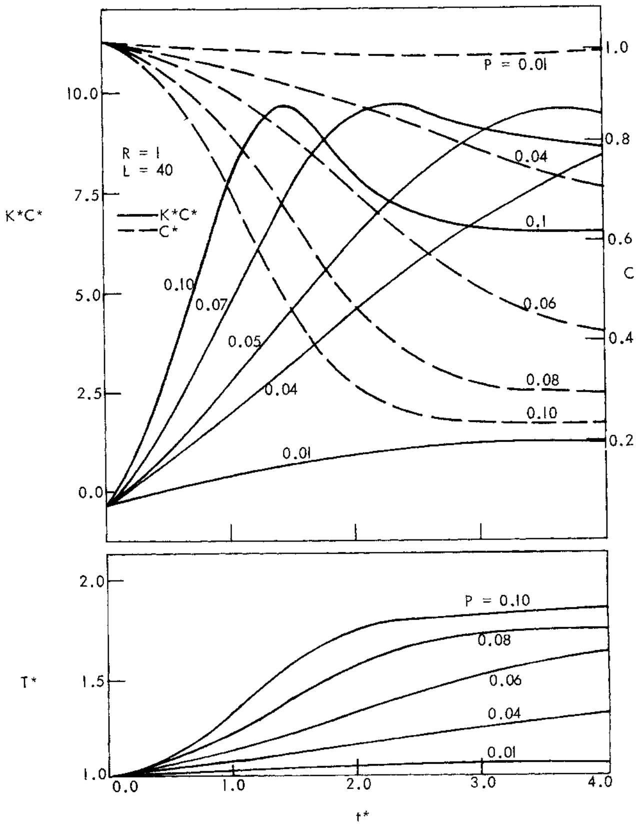

Fig. 7. Transient solution, effect of P on CST adiabatic operation.

solutions of the coupled nonlinear first-order differential equations are not feasible. Plots of these results are shown in Figures 6 and 7. The effect of the RL product is shown in Figure 6, and the effect of the relative time parameter P is shown in Figure 7. During the transient operation, C^* and K^* and thus r depend on the product RL, as has also been shown for steady state operation. This is shown by combining the transient equations and thereby obtaining one second-order differential equation in which R and L always occur in combination. For a given RL, r attains larger values during the transient operation than r at steady state only for values of P greater than P_{rm}.

It is interesting to note that the transient r goes through the maximum value $r_{\max}$ for values of P greater than P_{rm} only for the unrealizable case where the initial C^* is 1. This is shown in Figure 8, which shows the effect of the initial concentration of A, C_0^*, in the reactor on the transient behavior for fixed P and RL.

Semibatch Operation (SBO)

The basic equations for variable-volume operation for the adiabatic cases are

$$\frac{dC^*}{dt^*} = \frac{Q_f^*}{V^*}(1 - C^*) - PK^*C^* \tag{45}$$

$$\frac{dT^*}{dt^*} = \frac{Q_f^*}{V^*}(1 - T^*) + RPK^*C^* \tag{46}$$

$$K^* = 1 + L(T^* - 1) \tag{47}$$

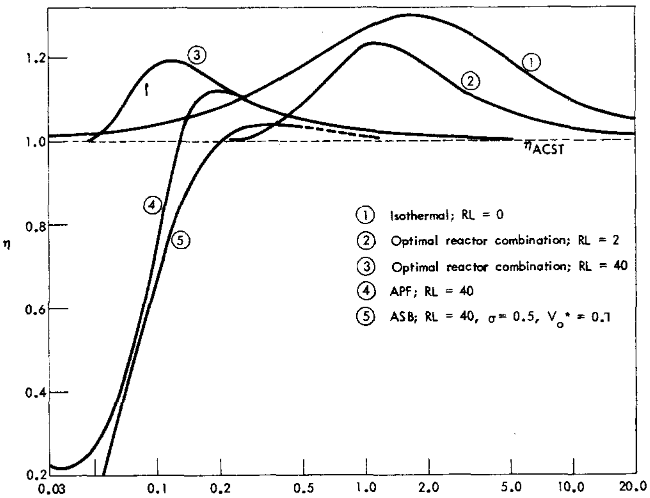

Fig. 9. Effect of relative time parameter P on relative SBO adiabatic yield.

$$V^* = V_0^* + \int_0^{t^*} (Q_f^* - Q^*)dt^* \tag{48}$$

In solving these equations it is desired to correlate η with a specified VVO policy and with the dimensionless parameters R, L, and P. As in the isothermal case, it is appropriate to compare the VVO yield to that of a CST with the same maximum volume and throughput rate.

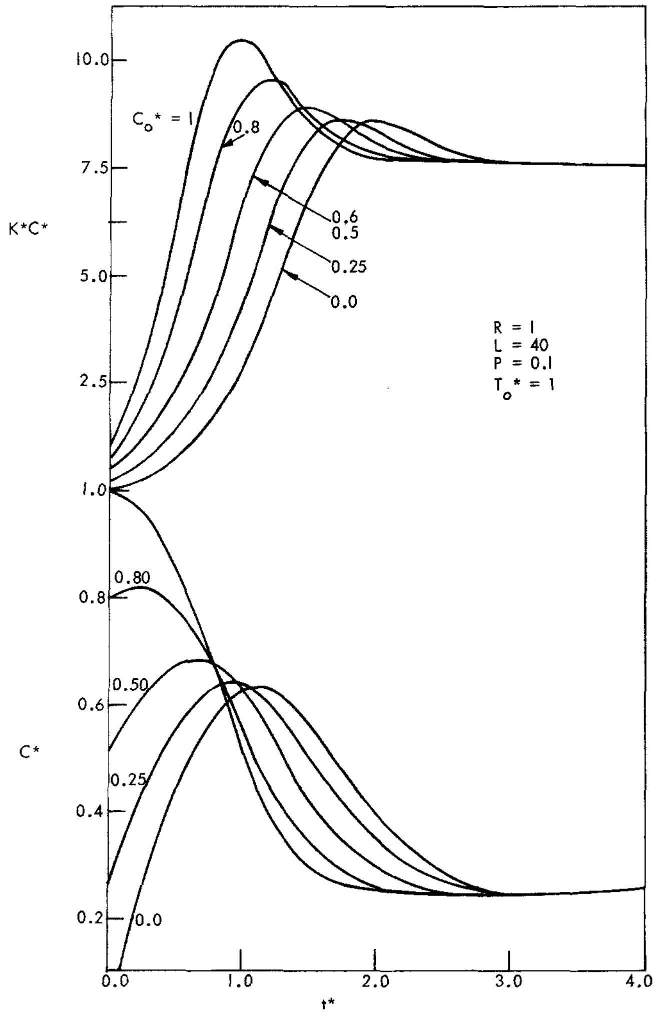

Fig. 8. Effect of initial concentration on adiabatic CST operation.

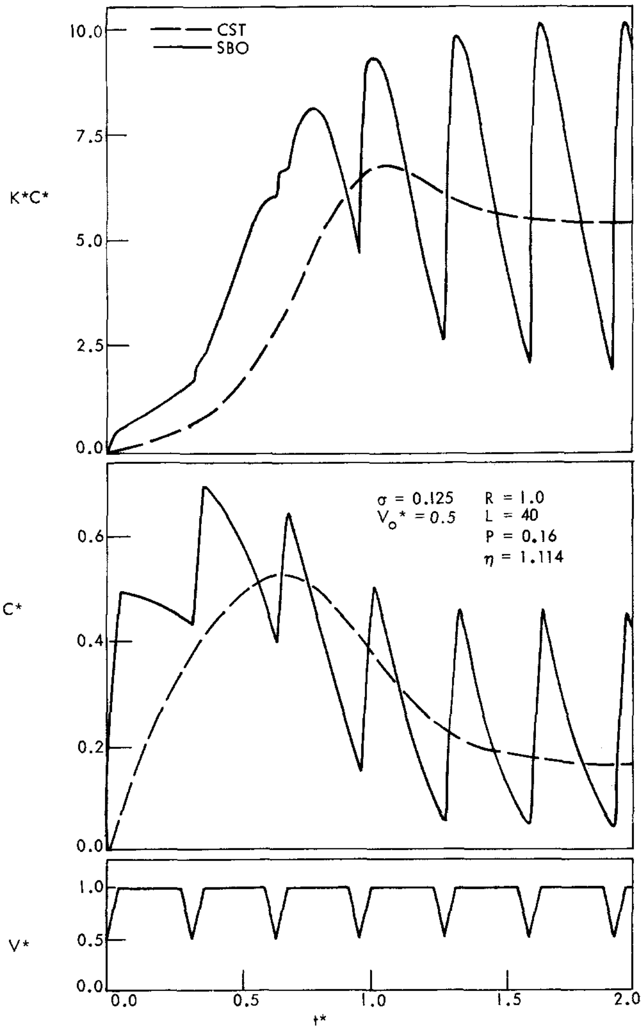

Fig. 10. Yield increase with SBO operation, adiabatic operation.

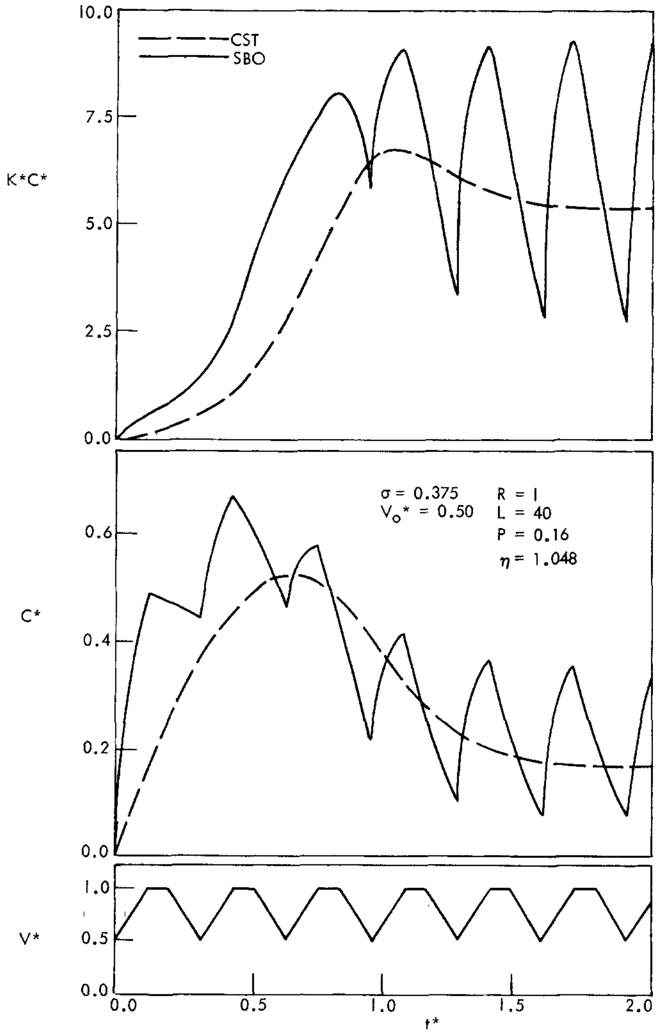

Fig. 11. Yield increase with SBO operation, adiabatic operation.

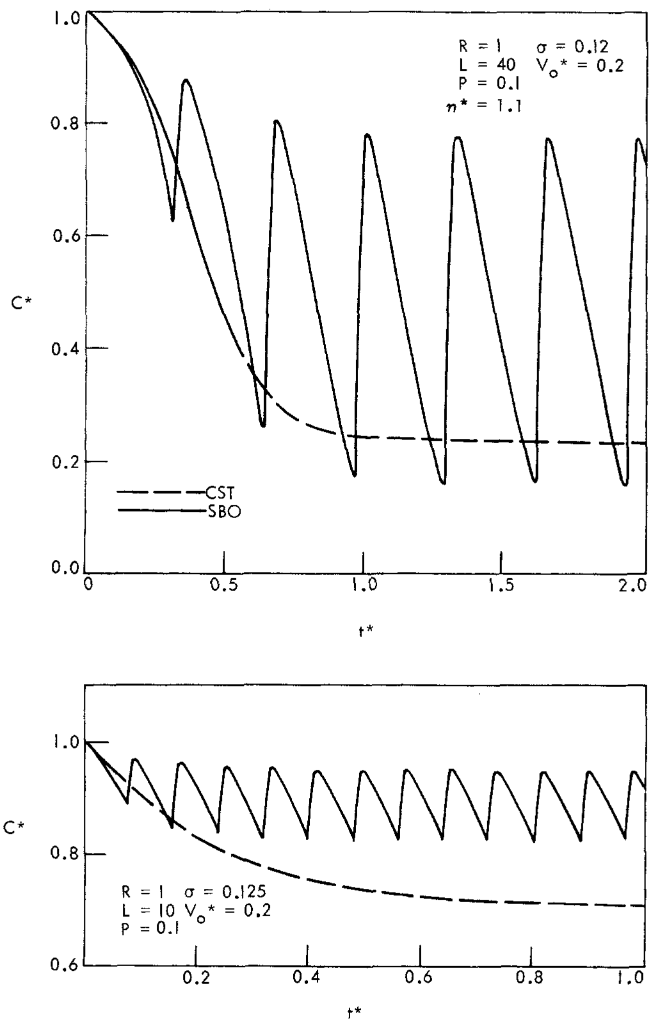

Fig. 12. SBO yield decrease due to change in *L*.

Many VVO policies could be considered. The SBO policy is considered here and is compared with SBO for the isothermal case. Results from SBO may be generalized qualitatively to more sophisticated VVO policies.

The operation policy to test the adiabatic reactor for semibatch operation was identical to that used for the isothermal case described earlier. A digital logic expansion system, the EAI DES-30, was used to operate the TR-48 analogue computer cyclically to simulate the SBO operation. The results of these computations are partially shown in Figures 9 to 12. The results are in part similar to those obtained for the isothermal case; that is, the relative yield η is a function of the fractional filling time, the relative time parameter P, the initial volume V_0^*, and in addition the parameters R and L, which do not occur in the isothermal case.

Figure 9 gives the relative yield [defined in Equation (27)] with respect to the adiabatic CST for the upper limit of adiabatic SBO and for a case of adiabatic SBO (ASBO) which approaches a lower limit of operation. The relative yield is shown as a function of P with RL as a parameter. Figure 9 corresponds to Figure 3 for the isothermal case. As in steady state operation, R and L appear in combination. The upper limit of ASBO is the optimal combination of an adiabatic CST and an adiabatic PFR. The optimal combination (curve 2) depicts an ACST operated at the conversion corresponding to the maximum reaction rate followed by an adiabatic PFR to bring the conversion to the desired value. Then SBO would employ an adiabatic CST operating at the maximum reaction rate followed by an adiabatic semibatch reactor. Figure 9 shows that the maximum attainable relative yield decreases as RL increases. That is, heat generation or a large temperature dependence has a detrimental effect on the maximum relative yield. Curve 4 in Figure 9 shows the well-known fact that for sufficiently exothermic reactions, the adiabatic CST gives a greater conversion than the adiabatic PFR at a small residence time and correspond-

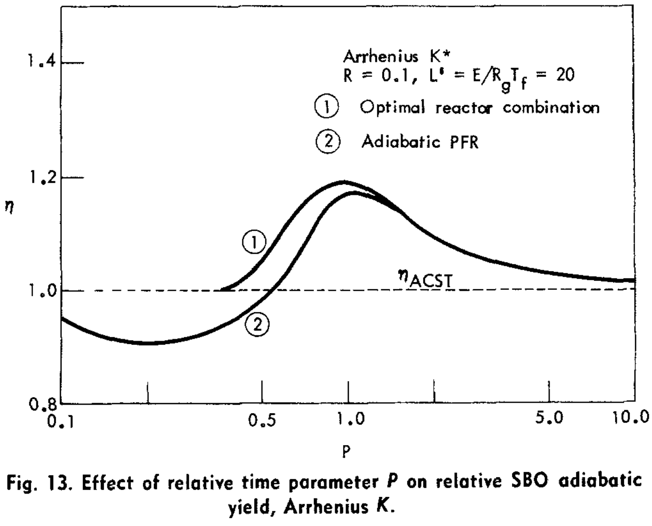

Fig. 13. Effect of relative time parameter *P* on relative SBO adiabatic yield, Arrhenius *K*.

ing low conversion. Curve 4 in Figure 9 shows that for sufficiently exothermic reactions, there is a range of residence time for which the relative yield for adiabatic operation is greater than the relative yield for isothermal operation.

Figures 10, 11, and 12 show examples of plots obtained from the analogue computer for adiabatic SBO. The dashed lines on the plots are the profiles from the CST case and the solid lines from the SBO case. The yield may be read directly from the plots, since

$$\eta_{CST} = 1 - C^* \qquad \eta_{SBO} = 1 - \overline{C^*} \tag{49}$$

where $\overline{C^*}$ is the average concentration in the reactor during the emptying stage. C^* is nearly linear during outflow, so the computation of $\overline{C^*}$ is easily performed, either on the computer or graphically. Figures 10 and 11, for different fractional filling times σ, show that, as in the isothermal case, the lower the filling time the higher the yield increase. The upper limit of relative yield is the batch reactor as discussed previously. Figure 12 demonstrates the effect of V_0^* and the parameter L on the cases treated in Figures 10 and 11. In Figure 12 the $L = 10$ SBO yield is less than that of the CST case.

The results given by Figure 9 will be valid only for a reactor system in which the temperature varies in small degree about the time average temperature. This is due to the expression of the reaction velocity constant as a linear function of temperature. Figure 13 shows a plot of relative yield for the upper limit of adiabatic SBO as a function of P in which the Arrhenius equation is used to express the temperature dependency of the reaction velocity constant. Curve 1 of Figure 13 is approximated by curve 2 of Figure 9.

The effect of the operating parameters of SBO on the relative yield will need further study. Specifically, the adiabatic SBO should be studied further by using the Arrhenius K. However, these initial investigations show that the SBO policy will decidedly result in yield increases for certain ranges of the parameters R, L, P, σ, and V_0^*.

SUMMARY

1. The transient and steady state operating equations for the isothermal variable-volume operation of a stirred tank reactor may be solved analytically for several limiting or approximate cases. The results may be used to predict behavior over ranges of operating conditions.

2. Semibatch operation of an isothermal reactor with first-order irreversible kinetics will result in relative yield increases over the constant volume case. The limiting relative yield increase, about 30%, corresponds to the case of a continuous flow reactor. The relative time parameter P affects the obtainable yield.

3. The isothermal semibatch equations may be solved analytically and used to predict behavior.

4. For the adiabatic case, the optimal CST constant volume operating conditions are unique functions of the parameters R, L, and P.

5. The transient solutions for the adiabatic CST are solved on an analogue computer and show the dependence on the parameters R, L, and P.

6. Semibatch operation will increase the yield over the CST case for adiabatic operation also, within certain ranges of the parameters R, L, P, V_0^*, and σ. The maximum yield increase for the adiabatic case is less than for the isothermal case. However, for sufficiently exothermic reactions and a large temperature dependence of the reaction velocity constant, the relative yield for the adiabatic case will be larger than for the isothermal case at small relative residence times.

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NOTATION

A = component being decomposed, $A \rightarrow B$
b = slope of $K(T)$
C_A = concentration of A, moles/vol.
C_{AF} = input concentration
C^* = C_A/C_{Af}
C_p = molal heat capacity of the liquid
H = dimensionless heat parameter
K = reaction rate constant, sec.$^{-1}$
L = relative rate parameter
P = relative time parameter
Q = output flow rate, vol./time
Q_f = input flow rate
Q_R = reference flow rate
q_s = heat loss to surroundings or coolant per unit volume
R = relative energy parameter
T = temperature
t = time
V = volume in the reactor
V^* = V/V_R
V_R = reference volume
$-\Delta H$ = heat of reaction
ρ = liquid density, moles/vol.
σ = relative filling time
η = relative yield

Subscripts

CST = continuous constant volume stirred tank reactor
CFR = continuous flow reactor
SBO = semibatch operation
VVO = variable-volume operation
PFR = plug flow reactor
0 = initial condition, time = 0
f = feed

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