R & D NOTES

Synchronized Periodic Operation of a Plug Flow Reactor and Bases of Comparison

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Periodic operation of chemical reactors has been the subject of numerous papers (Horn and Lin, 1967; Douglas, 1967; Lund and Seagrave, 1971; Codel and Engel, 1971; Chang and Bankoff, 1968; Kim and Hulbert, 1971; Bailey and Horn, 1971; Bailey, 1972, 1973). This note presents a mode of synchronized periodic operation involving flow and temperature for a plug flow reactor. A simple case of a single first-order reaction is treated to show that synchronizing periodic flow and temperature in a certain prescribed manner produces higher yield than any other modes of periodic operation considered under the constraints placed. In arriving at the results, bases for comparing various modes of unsteady periodic operation are derived from the constraints of equal throughput and heating requirement for all modes of periodic operation considered.

PERIODIC FLOW OPERATION

Transient periodic flow (TPF) operation is characterized as follows. First, feed rate to a plug flow reactor is intentionally and continuously alternated in a stepwise manner between higher and lower feed rate than the design rate. Second, magnitude of the step changes is bound by the constraint that throughput be the same in both periodic and nonperiodic operation. Third, duration of a step is one residence time of the reactant that enters the reactor when a step change is made. Completion of two step changes of one step-up to one step-down constitutes one cycle. Steady state, periodic flow (SPF) operation is different from the TPF operation in that the duration of a step is long enough for the operation to be considered at steady state. However, the ratio of the step-up period to the step-down period remains the same as in the TPF operation.

The constraint that the throughput be the same in both periodic and nonperiodic operation yields

$$v_o\tau = v_h\tau_h + v_l\tau_l \quad (\tau = \tau_h + \tau_l) \tag{1}$$

Dividing both sides of Equation (1) by v_o and using the definition of residence time, we have

$$\tau = 2\tau_o \quad \text{or} \quad 2\tau_o = \tau_h + \tau_l \tag{2}$$

Defining $r_h = v_o/v_h = \tau_h/\tau_o$ and $r_l = v_o/v_l = \tau_l/\tau_o$, we obtain from Equation (2)

$$r_h + r_l = 2 \tag{3}$$

PERIODIC TEMPERATURE AND SYNCHRONIZED OPERATION

In periodic temperature (PT) operation, reaction temperature is alternated in a stepwise manner between higher and lower temperature than the design isothermal value. Heating requirements for both periodic and nonperiodic operations are to be held the same. This condition bounds the magnitude of the step changes in temperature. As in

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the case of the TPF operation, completion of two step changes in temperature, one step-up and one step-down, constitutes one cycle. For convenience in combining the PT operation with the TPF operation, let the total time for one cycle be 2. Furthermore, let the duration of a step-down be represented by r_h and that of a step-up by r_l. Then, Equation (3) represents the relationship between r_h and r_l.

If we assume that the specific heat is constant, the constraint on the heating requirement dictates that

$$r_h T_c + r_l T_h = 2T \tag{4}$$

A simplified Arrhenius expression for the rate constant is

$$k' = k_o\, e^{a+bT} \tag{5}$$

and the expression, when solved for T, is

$$T = \frac{\ln(k'/k_o) - a}{b} \tag{6}$$

Substituting Equation (6) into Equation (4) and making use of Equation (3), we have

$$(k_c')^{r_h}(k_h')^{r_l} = (k')^2 \tag{7}$$

To obtain higher average yield, the step-up period (higher temperature) should be longer than the step-down period (lower temperature). Thus, duration of the step-down r_h will assume a value less than 1.

Synchronization of the TPF operation with the PT operation is shown in Figure 1 for the synchronized periodic operation. For the synchronized periodic operation, the feed rate also changes along with the reaction temperature, and the relationship of Equation (7) needs to be changed as follows:

$$k_c' k_h' = (k')^2 \tag{8}$$

We note in Figure 1 that low reaction temperature coincides with high feed rate.

AVERAGE YIELD OF A FIRST-ORDER REACTION FOR VARIOUS MODES OF PERIODIC OPERATION

For an isothermal and plug flow reactor where a first-order reaction occurs, the transient concentration when subjected to a change in feed rate can be represented by

$$r\frac{\partial x}{\partial t} + \frac{\partial x}{\partial z} = -krx \tag{9}$$

If the reactor is at steady state for a given feed rate corresponding to r_h, we have

$$x(z, o) = e^{-kr_h z} \tag{10}$$

If the feed rate changes from the rate corresponding to r_h to r_l at time zero, the exit concentration during the step-down period is

$$x(1, t) = e^{-kr_h(1-t/r_l)}e^{-kt} \tag{11}$$

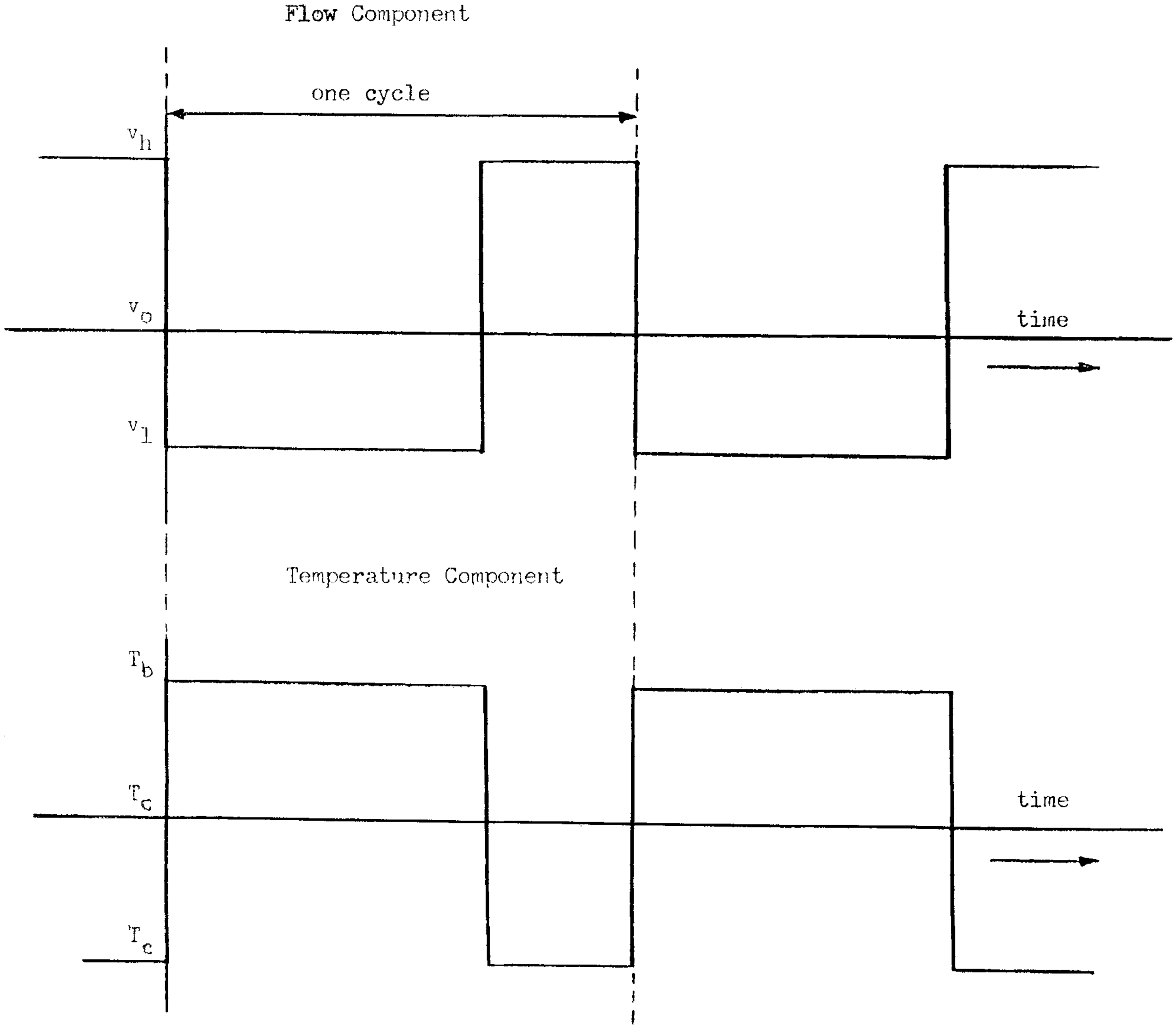

Fig. 1. Synchronized periodic operation.

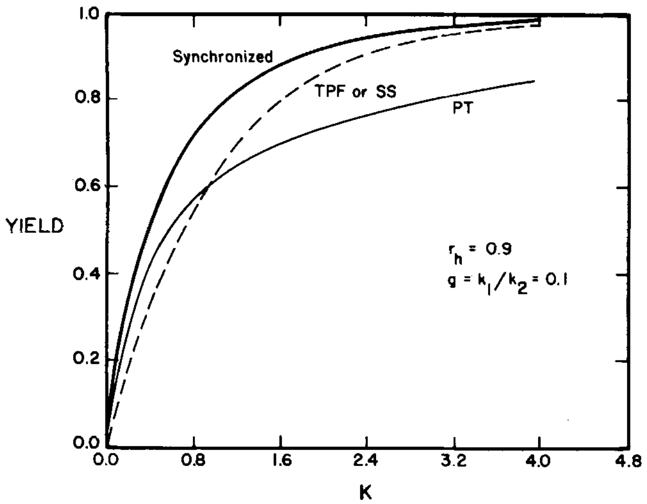

Fig. 2. Yield for synchronized operation and its components, periodic-temperature (PT) and transient periodic-flow (TPF) operation.

since the switching of the feed rate occurs at the exact time ($t = r_l$) that the reactor reaches the new steady state. Average concentration during the period can be obtained by

$$y = \frac{1}{r_l}\int_0^{r_l} x(1,t)\,dt \tag{12}$$

and the result is

$$y_t = \frac{e^{-kr_h} - e^{-kr_l}}{k(r_l - r_h)} \tag{13}$$

It can be shown that the average concentration for the step-up period is the same as the one given by Equation (13). Therefore, average concentration for one complete cycle is also represented by Equation (13). Average yield obtainable by various modes of periodic operation is summarized in Table 1.

TABLE 1. AVERAGE YIELD OBTAINABLE BY VARIOUS MODES OF PERIODIC OPERATION, YIELD = $1 - y$

Mode of operation	y
Steady state (SS)	e^{-k}
Periodic temperature (PT)	$\frac{r_h e^{-k_1} + r_l e^{-k_2}}{2}$
Steady state periodic flow (SPF)	$\frac{r_h e^{-kr_h} + r_l e^{-kr_l}}{2}$
Transient periodic flow (TPF)	$\frac{e^{-kr_h} - e^{-kr_l}}{k(r_l - r_h)}$
Steady state synchronized (S. Synchronized)	$\frac{r_h e^{-k_1 r_h} + r_l e^{-k_2 r_l}}{2}$
Synchronized	$\frac{e^{-k_1 r_h} - e^{-k_2 r_l}}{k_2 r_l - k_1 r_h}$

TABLE 2. k RELATIONSHIP FOR COMPARISON PURPOSES

Comparison pair	Relationship for k
S. synchronized or synchronized vs. SS, SPF, or TPF	$k = \sqrt{k_1 k_2}$
TP vs. SS, SPF, or TPF	$k = k_1^{r_h/2}\, k_2^{r_l/2}$
TP vs. S. synchronized or synchronized	$k = k_1^{r_h/2}\, k_2^{r_l/2}$ for TP $k = \sqrt{k_1 k_2}$ for S. synchronized or synchronized

In comparing various modes of operation, care should be taken to ensure proper conversion of the normalized rate constants [Equations (7) and (8)]. Summarized in Table 2 are the relationships to be used in comparing various modes of operation. The rate constants k_1 and k_2 in Table 2 include the steady state residence time, k_1 corresponding to k_c' and k_2 to k_h'. Therefore, we have in terms of k

$$k^2 = k_1^{r_h} k_2^{r_l} \quad \text{in place of Equation (7)} \tag{14}$$

and

$$k^2 = k_1 k_2 \quad \text{in place of Equation (8)} \tag{15}$$

Yield curves for various modes are shown in Figure 2. The results are for $r_h = 0.9$ (11% increase in throughput over the design value during the step-up period) and $k_1/k_2 = 0.1$. It is shown that the synchronized periodic operation improves yield significantly over the entire yield range, whereas each component (PT and TPF) of the operation shows no improvement (TPF), and relatively small improvement in the low yield range and significant deterioration in the high yield range (PT). Yield curve for the steady state synchronized operation (SPF + PT) closely follows the yield curve of the PT operation. It is notable that the TPF operation results in lower yield than the yield obtainable by steady state operation.

TWO PARALLEL STEADY STATE REACTORS AND PERIODIC OPERATION

Periodic operation necessarily requires averaging in arriving at a value of the quantity of interest. That value can certainly be obtained by mixing the outputs of two parallel processes operating at steady state. For any comparison to be meaningful, there has to be a basis for comparison. Since all the periodic operations considered here were compared with the result obtainable by one steady state, plug flow reactor, we compare the result of one steady state reactor with that of two steady state reactors based on equal volume and equal throughput. Comparison between periodic operation of one reactor and two steady state reactors in parallel can then be made through one steady state reactor as the reference. The conditions of equal volume and throughput for both cases yield

$$V_o = V_l + V_h \tag{16}$$

$$F_o = F_l + F_h \tag{17}$$

The two equations can be combined into

$$1 = \frac{t_o}{t_l} R + \frac{t_o}{t_h}(1 - R) \tag{18}$$

and the resulting average concentration for a first-order reaction becomes

$$y_2 = \left\{ 1 - \frac{t_o}{t_h}(1 - R) \right\} e^{-t_l k} + \frac{t_o}{t_h}(1 - R)\, e^{-t_h k} \tag{19}$$

Actual computation of Equation (19) with the constraint of Equation (18) for the yield shows that yield obtainable by a single steady state, plug flow reactor is always higher than the yield obtainable by two steady state, plug flow reactors in parallel.

NOTATION

a, b = constants in simplified Arrhenius expression
F_o, F_h, F_l = volumetric flow rate of reference reactor, that

of larger reactor and that of small reactor in two parallel reactor scheme

k = rate constant combined with residence time, $k'\tau_o$

k', k_o = rate constant and preexponential factor

k_c', k_h' = rate constant corresponding to T_c and T_h

k_1, k_2 = $k_c'\tau_o$ and $k_h'T_o$, respectively

r = inverse of velocity normalized with respect to v_o, v_o/v

r_h = duration of normalized step-up period for periodic flow operation, inverse of normalized velocity during step-up period

r_l = duration of normalized step-down period for periodic flow operation, inverse of normalized velocity during step-down period

R = V_l/V_o

t = time normalized with respect to τ_o

t_o, t_h, t_l = residence time in two parallel reactor scheme; V_o/F_o, V_h/F_h and V_l/F_l

T, T_h, T_c = design operating temperature, feed temperature during step-down period and during step-up period

v_o, v_h, v_l = design feed velocity, velocity during step-up period and during step-down period

V_o, V_h, V_l = volume of reference reactor, that of larger reactor and that of smaller reactor in two parallel reactor scheme

x = normalized concentration of A, A/A_o

y = average value of x $(1, t)$

y_t = y for TPF operation

z = distance normalized with respect to reactor length

τ_h = duration of step-up period, residence time corresponding to v_h

τ_l = duration of step-down period, residence time corresponding to v_l

τ_o = residence time corresponding to v_o

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Manuscript received July 29, 1977; revision received January 3, and accepted January 5, 1978.

Heat Transfer in Plane Couette Flow with Additional Pressure Gradient Including Entrance Effects for a Non-Newtonian Fluid

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Analytical solutions are presented for laminar plane Couette flow of a power law non-Newtonian fluid. Effects of an additional negative pressure gradient were included in solving for the velocity distribution. The contributions due to the entrance heating region and the viscous dissipation effects were included in arriving at the temperature distribution and also the variation of the local Nusselt number at the stationary plate.

Heat transfer in plane Couette flow has been given due attention because of some important applications as pointed out by Bruin (1972). One example of such applications is the study of thermal pasteurization processing of liquid foods. As suggested by Bruin (1972), the death rate of microorganisms can be considered as a first-order chemical reaction, where the reaction constant is strongly temperature dependent. Another example is the extrusion of the paper pulp prior to rolling on the paper machines. Liquid foods or paper pulp are, in general, non-Newtonian, and therefore an analysis considering this fact would be more accurate than those found in the published work by Bruin (1972), Sestak and Rieger (1969), El-Ariny and Aziz (1976), and Hudson and Bankoff (1965). Tien (1961) considered the case of simple Couette flow of a non-Newtonian power law fluid; however, his solution is good only for fully developed velocity and temperature profiles. Tien (1962) also extended the Graetz-Nusselt problem to non-Newtonian fluids, and Suckow et al. (1971) improved on it. However, these two solutions were for the case of two stationary plates, and it may not be suitable to compare them with the present work.
