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Intermediate Storage in Noncontinuous Processes Involving Stages of Parallel Units

A model is developed to study holdup in intermediate storage as a function of system parameters such as processing unit delay times. General results concerning the periodicity of the required storage volume, the allowable unit delay times, and the calculation of the volume are presented. Analytical expressions for the limiting volume are obtained for several special network configurations. A simple upper bound is derived for purposes of quick estimates of the limiting volume for the general case, and a gradient based algorithm is reported for obtaining the minimum volume schedule for general networks.

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SCOPE

Intermediate storage is widely used in batch and semicontinuously operated plants to increase plant availability, dampen the effects of process fluctuations, reduce process cycle times, and provide flexibility in sequencing and scheduling. These roles have only recently begun to be subjected to systematic study. Oi et al. (1977) considered the optimal scheduling and sizing of intermediate storage in a waste treatment plant. Takamatsu et al. (1979) treated a case of storage intermediate to one continuous and *M* parallel batch units. Oi (1982) examined the problem of schedule revision to accommodate nonperiodic flow fluctuations, while Takamatsu et al. (1982) presented an analysis of the minimum storage for several cases of the serial batch-batch configuration. Finally, Karimi and Reklaitis (1983) developed analytical result for the limiting storage volume in serial systems composed of arbitrary configurations of batch, semicontinuous, or continuous operations.

This paper extends the analysis of the predecessor paper to periodically operated networks composed of a set of parallel units followed by intermediate storage followed by another set of parallel units. We begin with a Fourier series formulation of the network model, continue with the development of the periodicity properties of the storage volume, and then develop formulas for calculating the required storage volume, given the unit delay times, capacities, and flow rates. Next, simplified results are obtained for several special cases involving identical units including some previously considered in the literature. The paper concludes with the development of an efficient algorithm for determining the unit delay time schedule which minimizes the required storage volume.

CONCLUSIONS AND SIGNIFICANCE

A comprehensive analysis of the deterministic periodically operated parallel unit case was presented. The analytical expressions derived for the limiting storage volume required to decouple the upstream and downstream processing stages are quite simple and obviate the need for simulation. The special, but common, case involving identical parallel units and periodic operation with symmetrically spaced delay times was shown to be equivalent to the one-one serial case for which analytical results were reported earlier. A simple bound on the required volume is also derived for the general *L-M* case. The important result, giving the characteristic period of the storage volume with respect to the delay time of a given unit, generalizes results previously reported for special cases and significantly reduces the search interval for finding the optimum periodic operating

schedule. Finally, a gradient-based search method for determining the optimum schedule was developed using the one-sided derivatives of the holdup function and was shown to be superior to conventional direct search for solving the storage minimization problem.

This work constitutes a further step towards the achievement of rational ways of sizing intermediate storage vessels which can replace the reliance on experience and rules of thumb. The results presented cover most of the configurations of noncontinuous processes commonly found in practice. The results can be effectively used in the the studies of the optimal division of long processing trains into subprocesses separated by intermediate storage tanks. Conventional design procedures for noncontinuous processes, which usually neglect the existence of intermediate storage both in calculating operating parameters and in evaluating the system cost, can be considerably improved by incorporating the general results of this paper. Although no explicit consideration was given in our analysis to the processing of multiple products, many commonly occurring processing patterns involving multiple products can readily be treated as extensions of the single product case.

MATHEMATICAL MODEL OF THE PROCESS

Assumptions

A schematic diagram of the process under consideration is shown in Figure 1. As shown in the figure, both stages employ batch/continuous/semicontinuous units with L units in the upstream stage and M in the downstream stage. V^* is the size of the storage vessel; V_i is the batch size of ith unit; ω_i is the cycle time of ith unit. The basic assumptions, underlying the mathematical model, are as follows:

1 Semicontinuous units process material in batches of fixed sizes at constant rate. After processing a fixed amount of material, they remain idle for a fixed interval of time and then resume operation in a periodic manner.

2. Batch units operate with fixed batch sizes and fixed cycle times. A typical cycle of a batch unit consists of operations such as firing, processing, emptying, and preparation and/or waiting.

3. The productivities of both stages are equal, i.e.

$$\sum_{i=1}^{L} V_i/\omega_i = \sum_{i=L+1}^{N} V_i/\omega_i$$

where N is the total number of units, $L + M$.

4. There exist least integers β_i, $i = 1,N$; such that $\beta_i\omega_i = \beta_j\omega_j$; $\forall\ i,j$. This essentially amounts to stating that a cycle time ω_i can as an engineering approximation be rounded off to a rational number. This in turn assures the existence of an extended least common multiple (LCM) of $\omega_1,\omega_2, \ldots ,\omega_N$, denoted by $\Omega = \mathrm{LCM}(\omega_1,\omega_2, \ldots ,\omega_N) = \beta_i\omega_i, \forall i$.

5. The discharge rates of all the upstream units and the feed rates of all the downstream units, although different, are constant and known.

6. The batch sizes, the flow rates, and the storage size are all in the same units, i.e., either mass or volume.

7. The required size of the storage tank is equal to the maximum holdup in the tank.

Formulation

We will present here a general formulation for a two-stage system with parallel, nonidentical units and an intermediate storage tank. A system consisting of L upstream parallel units followed by a storage vessel followed by M downstream, parallel units will be referred to as an L-M system. In this notation, a serial system is denoted as a 1-1 system.

The cycle time of a batch unit, ω, is given by $\omega = T_f + T_B + T_e + T_P$. The cycle time of a semicontinuous unit, ω, is similarly given by $\omega = T_S + T_i$.

For every batch unit, we define a characteristic fraction x, called an emptying or a filling fraction, as follows:

$$x_i = (T_e)_i/\omega_i \text{ or } x_j = (T_f)_j/\omega_j \qquad (1a,b)$$

The units in the upstream stage are characterized by emptying fractions, while those in the downstream stage by filling fractions. For semicontinuous units, we define a similar quantity, which is equivalent to a processing fraction, as

$$x_i = (T_S)_i/\omega_i \qquad (1,c)$$

Let us denote the flow rate for a unit as U_i. For upstream units U_i is equal to the discharge rate, while for downstream units it is equal to the feed rate. From the definition of batch size for a unit, V_i is either $U_i(T_e)_i$ or $U_i(T_f)_i$ or $U_i(T_S)_i$ in accordance with the type of unit and the stage where it is located. Consequently,

$$V_i = U_i x_i \omega_i \qquad (2)$$

To each unit i, we assign a characteristic flow function, $F_i(t)$, as:

$$F_i(t) = \begin{cases} c_i U_i & \alpha\omega_i \le t \le \alpha\omega_i + x_i\omega_i \\ 0 & \alpha\omega_i + x_i\omega_i < t < (\alpha + 1)\omega_i \end{cases}$$

where, α is an integer and coefficients c_i are defined as:

$$c_i = \begin{cases} +1 \text{ if } i\text{th unit is an upstream unit} \\ -1 \text{ if } i\text{th unit is a downstream unit} \end{cases} \qquad (3)$$

We arbitrarily select as the origin of time, the time when the storage tank commences to be filled from unit 1. The starting moments for the upstream units are defined as the moments when they start discharging material into the storage tank, while those for the downstream units are defined as the moments when they commence being filled by the storage vessel. We also take the starting moment of unit 1 or equivalently the origin as the reference point for determining the delay of starting moments for all other units. Now, if $t_i \ge 0$ is the first starting moment of the unit i, we define the fractional delay time variable y_i as:

$$y_i = t_i/\omega_i \qquad (4)$$

As $F_i(t)$ has a period of ω_i, y_i must satisfy $0 \le y_i < 1$. Furthermore, we define the fractional delay time vector $Y = (y_1,y_2,y_3, \ldots ,y_N)$. Clearly, from the definition of delay time, $y_1 = 0$ always. Finally, the holdup in the intermediate storage vessel, $V(t)$, is described by:

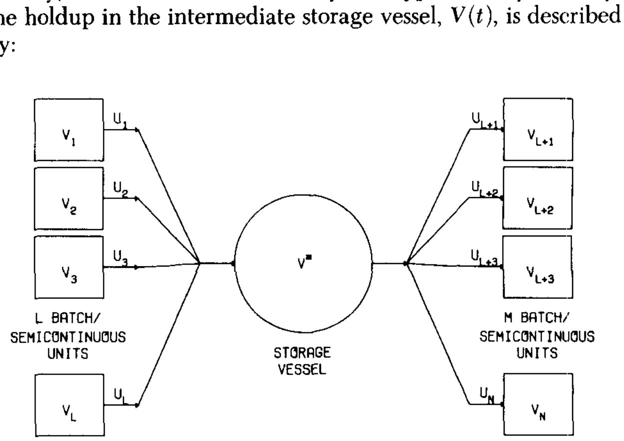

Figure 1. Schematic diagram of the process.

$$\frac{dV(t)}{dt} = \sum_{i=1}^{N} F_i(t - t_i) \quad (5)$$

Therefore,

$$V(t) = V(0) + I(t) \quad (6)$$

where,

$$I(t) = \int_0^t \sum_{i=1}^{N} F_i(\tau - t_i) d\tau \quad (7)$$

Defining

$$V_{\max} = \overset{\max}{t} I(t) \text{ and } V_{\min} = \overset{\min}{t} I(t) \quad (8a,b)$$

it follows from Eq. 5 that,

$$\overset{\max}{t} V(t) = V(0) + V_{\max} \text{ and } \overset{\min}{t} V(t) = V(0) + V_{\min} = 0$$

since negative holdup is not feasible. Hence, from assumption 7,

$$V^* = V_{\max} - V_{\min} \quad (9)$$

To express the discontinuous function $F_i(t)$ compactly, we resort to Fourier series (Tuma, 1979). One can easily verify that,

$$F_i(t) = c_i \left[\frac{V_i}{\omega_i} + \sum_{n=1}^{\infty} \frac{2U_i}{n\pi} \sin n\pi x_i \cos 2n\pi \left(\frac{t}{\omega_i} - \frac{x_i}{2}\right)\right] \quad (10)$$

The function $F_i(t)$ satisfies the conditions of Dirichlet's theorem (Sokolnikoff and Redheffer, 1974) and hence, the above Fourier series is convergent and represents $F_i(t)$. The following lemma is a prerequisite to further analysis.

Lemma I. Any Fourier series (whether convergent or not) can be integrated term by term between any limits. The integrated series converges to the integral of the periodic function corresponding to the original series (Sokolnikoff and Redheffer, 1974).

With the help of Lemma-I, assumption 3 and Eqs. 5, 6 and 9, one can show the following proposition.

Proposition I. The holdup in the intermediate storage vessel, $V(t)$, is given by:

$$V(t) = V(0) + \sum_{i=1}^{N} \sum_{n=1}^{\infty} \frac{c_i U_i \omega_i}{n^2\pi^2} \sin n\pi x_i \left[\sin 2n\pi\left(\frac{t}{\omega_i} - y_i - \frac{x_i}{2}\right) + \sin 2n\pi\left(y_i + \frac{x_i}{2}\right)\right]$$

Note that the holdup in the intermediate storage vessel, $V(t)$, is a periodic function with period Ω. As a consequence, the maximization and minimization of Eqs. 8a and 8b can be confined to the range $0 \le t \le \Omega$.

ANALYSIS OF GENERAL *L-M* SYSTEM

Periodicity of $V^*(y)$

For purposes of this section only, we relax assumptions 1, 2 and 5. Thus we consider a general *L-M* system involving arbitrary processing characteristics and arbitrary feed or discharge rates, with $c_i f_i(t)$ denoting the characteristic flow rate function of unit i and c_i as defined in Eq. 3, but we generalize the definition of "batch size" V_i as

$$V_i = \int_0^{\omega} f_i(t) dt$$

As before, the units operate periodically with their starting moments delayed by their respective delay times. We state the following general result (proof given in Appendix I) concerning the periodic behavior of the size of the storage vessel.

Theorem I. Let $f_i(t)$, $i = 1,N$ be arbitrary, periodic input or output flow rates of an intermediate storage vessel subject to the following:

1. Each $f_i(t)$ satisfies the conditions of Dirichlet's theorem (Sokolnikoff and Redheffer, 1974).
2. $\sum_{i=1}^{N} c_i V_i/\omega_i = 0$
3. Holdup in the intermediate storage vessel is given by:

$$\frac{dV(t)}{dt} = \sum_{i=1}^{N} c_i f_i(t - t_i)\, t_1 = 0$$

Then, the size of the storage vessel $V^*(Y)$ is a periodic function with respect to y_j, while keeping $y_i, i \neq j$ fixed; and the period is $1/g_j$ where $g_j = GCM(\beta_1, \beta_2, \ldots, \beta_{j-1}, \beta_{j+1}, \ldots, \beta_{N-1}, \beta_N)$.

This theorem generalizes the results reported by Takamatsu et al. (1979) for the *L*-1 and 1-*M* case involving *L* or *M* batch and 1 continuous unit. The practical importance of the result lies in the significant reduction of the range of y_i which must be searched to obtain a set of y_i which minimize $V^*(Y)$. In addition, notice that it is the function $V^* = V_{\max} - V_{\min}$ which is periodic and not $V_{\max}$ and $V_{\min}$ separately. This is important since $V(0) = -V_{\min}$ and thus $V_{\min}$ indicates the initial inventory $V(0)$, with which one should start the periodic operation. Hence, although the choice of y_j or $y_j + 1/g_j$ as fractional delay time requires the same storage size, the initial inventories required for both choices are different. Clearly, this freedom in the choice of y_j, helps one in picking the most "suitable" delay time for every unit.

Sizing Procedure

In the subsequent discussion, we restore assumptions 1, 2 and 5, and proceed to develop expressions leading to the required size of the intermediate storage tank for the *L-M* system,

From Eq. 6 and Proposition I, we obtain,

$$I(t) = \sum_{i=1}^{N} \sum_{n=1}^{\infty} \frac{c_i U_i \omega_i}{2n^2\pi^2} \left[\cos 2n\pi(u_i - z_i) - \cos 2n\pi z_i - \cos 2n\pi(u_i - y_i) + \cos 2n\pi y_i\right] \quad (11)$$

where,

$$z_i = \text{mod}(x_i + y_i, 1) \quad (12)$$

and

$$u_i = \text{mod}(t/\omega_i, 1) \quad (13)$$

The above expression for $I(t)$ can be further simplified by using the relation (Tuma, 1979),

$$\sum_{n=1}^{\infty} \frac{\cos 2n\pi\vartheta}{n^2\pi^2} = 1/6 - |\vartheta| + \vartheta^2 \qquad |\vartheta| \le 1 \quad (14)$$

thus obtaining the following proposition.

Proposition II. For a general *L-M* system,

$$I(t) = \sum_{i=1}^{N} \frac{1}{2} c_i U_i \omega_i h(u_i, y_i, z_i)$$

where, $h(u_i, y_i, z_i) = |u_i - y_i| - |u_i - z_i| + (2u_i - 1)(y_i - z_i)$.

The following lemma is a direct consequence of the piecewise constant nature of the derivative of $V(t)$.

Lemma II. $V(t)$ is a piecewise linear function with corner points representing its multiple optima.

From the periodicity of $V(t)$, attention needs to be focused only on the range, $0 \le t < \Omega$. It is easy to see that the set of aforementioned corner points, denoted as T, is:

$$T = [t_{ij} : t_{ij} = i\omega_j + y_j\omega_j \text{ or } t_{ij} = i\omega_j + (x_j + y_j)\omega_j; 0 \le i \le \beta_j - 1; 1 \le j \le N]$$

We can further divide T into two subsets such that

$$T_{\max} = [t_{ij} : t_{ij} \epsilon T; t_{ij} \text{ is a candidate for } I(t_{ij}) = V_{\max}]$$

$$T_{\min} = [t_{ij} : t_{ij} \epsilon T; t_{ij} \text{ is a candidate for } I(t_{ij}) = V_{\min}]$$

One can show that $T_{\max}$ and $T_{\min}$ are defined as given by the following lemma.

Lemma III. $T_{\max}$ and $T_{\min}$ are

$$T_{\max} = [t_{ij} : t_{ij} = i\omega_j + (x_j + y_j)\omega_j, 1 \le j \le L \text{ or } t_{ij} = i\omega_j + y_j\omega_j, L + 1 \le j \le N, 0 \le i \le \beta_j - 1]$$

$$T_{\min} = [t_{ij}: t_{ij} = i\omega_j + (x_j + y_j)\omega_j, L + 1 \le j \le N \text{ or } t_{ij} = i\omega_j + y_j\omega_j, 1 \le j \le L, 0 \le i \le \beta_j - 1]$$

Now it is clear that using Eqs. 6 and 9, one can obtain V^* by evaluating,

$$V_{\max} = \max_{t_{ij}\in T_{\max}} I(t_{ij}) \text{ and } V_{\min} = \min_{t_{ij}\in T_{\min}} I(t_{ij}) \quad (15a,b)$$

In fact, it is easy to recognize that the $t_{ij}\in T$ would represent the event times in an event-oriented discrete simulation of the system of Figure 1. However, Eq. 15 show that it is not necessary to resort to a full-fledged simulation to evaluate V^*, since $I(t_{ij})$ can be readily calculated without the knowledge of its values at other t_{ij}'s. Instead it is sufficient to evaluate $I(t)$ at $2\sum_{j=1}^{N}\beta_j$ points to determine the size of the storage vessel. However, as we shall see in the next section, one can reduce the number of evaluations of $I(t)$ considerably in cases involving identical units.

SYSTEMS WITH IDENTICAL UNITS

In this section, we consider two common configurations involving identical processing units. The first case is the 1-*M* or *L*-1 system. The second case is the *L*-*M* configuration in which each stage consists of identical units and the starting moments of the units in a stage are delayed by equal intervals.

First, we consider the 1-*M* system. Clearly, $\beta_2 = \beta_j, \omega_2 = \omega_j, V_2 = V_j, U_2 = U_j, x_2 = x_j$ for $2 \le j \le M + 1$. As shown in the analysis of the general case, one would be required to evaluate $I(t)$ at $2(\beta_1 + M\beta_2)$ points to obtain the tank size. However, we will show that for the configuration under consideration, the number of evaluations can be reduced to $2(\beta_1 + M)$ points. This is accomplished by analytically derived expressions for an upper bound for $V_{\min}$ and a lower bound for $V_{\max}$ from the subsets of $T_{\min}$ and $T_{\max}$, respectively. These subsets are

$$T'_{\min} = [t_{ij}: t_{ij}\in T_{\min};\ t_{ij} = i\omega_2 + (x_2 + y_j)\omega_2;\ 0 \le i \le \beta_2 - 1; 2 \le j \le M + 1]$$

$$T'_{\max} = [t_{ij}: t_{ij}\in T_{\max};\ t_{ij} = i\omega_2 + y_j\omega_2;\ 0 \le i \le \beta_2 - 1; 2 \le j \le M + 1]$$

The analytical procedure involved in evaluating $I(t_{ij})$ for $t_{ij}\in T'_{\min}$ or $t_{ij}\in T'_{\max}$ resembles that employed in the analysis of the 1-1 system (Karimi and Reklaitis, 1983). Furthermore, let $m = \omega_1/\omega_2 = \beta_2/\beta_1$, $p = 1/\beta_1$, $p' = 1/\beta_2$ and $\delta_1 = \text{mod}(mx_1,p)$.

Proposition IIIa. For a 1-*M* system with identical units,

$$\max_{t_{ij}\in T'_{\max}} I(t_{ij}) = \max_{2 \le j \le M+1}\left\{V_1(1 - x_1) + \frac{V_1}{m}\left(\frac{S_{\max}}{x_1} - y'_j\right) - \frac{1}{2}U_2\omega_2\sum_{k=2}^{M+1} h(z_j,y_k,z_k)\right\}$$

$$\min_{t_{ij}\in T'_{\min}} I(t_{ij}) = \min_{2 \le j \le M+1}\left\{\frac{V_1}{M}\left(\frac{S_{\min}}{x_1} - z'_j\right) - \frac{1}{2}U_2\omega_2\sum_{k=2}^{M+1} h(z_j,y_k,z_k)\right\}$$

where $S_{\max} = \max[0,y'_j - p(1 - x_1)]$, $S_{\min} = [z'_j,px_1]$, $y'_j = \text{mod}(y_j - \delta_1,p)$ and $z'_j = \text{mod}(z_j,p)$.

From this result and Eqs. 15a,b, it is clear that one needs $2(\beta_1 + M)$ evaluations of $I(t)$ to obtain V^*.

For an *L*-1 system, we have $\beta_1 = \beta_j$, $\omega_1 = \omega_j$, $V_1 = V_j$, $U_1 = U_j$, and $x_1 = x_j$ for $1 \le j \le L$. To obtain V^* for this system, it suffices to evaluate $I(t)$ at $2(\beta_{L+1} + L)$ points as compared to $2(\beta_{L+1} + L\beta_1)$ points for the general case. The subsets $T_{\min}$ and $T_{\max}$ for this system are

$$T'_{\max} = [t_{ij}: t_{ij}\in T_{\max};\ t_{ij} = i\omega_1 + (x_1 + y_j)\omega_1;\ 0 \le i \le \beta_1 - 1; 1 \le j \le L]$$

$$T'_{\min} = [t_{ij}: t_{ij}\in T_{\min};\ t_{ij} = i\omega_1 + y_j\omega_1;\ 0 \le i \le \beta_1 - 1; 1 \le j \le L]$$

Also, we define $p = 1/\beta_{L+1}$, $p' = 1/\beta_1$, $m = \omega_{L+1}/\omega_1 = \beta_1/\beta_{L+1}$ and $\delta_{L+1} = \text{mod}(mx_{L+1},p)$. Then, the equivalent of Proposition IIIa for an *L*-1 system can be stated as follows.

Proposition IIIb. For an *L*-1 system with identical units,

$$\max_{t_{ij}\in T'_{\max}} I(t_{ij}) = \max_{1 \le j \le L}\left\{\frac{V_{L+1}}{m}\left(my_{L+1} + z'_j - \frac{S_{\min} + ms}{x_{L+1}}\right) + \frac{1}{2}U_1\omega_1\sum_{k=1}^{L} h(z_j,y_k,z_k)\right\}$$

$$\min_{t_{ij}\in T'_{\min}} I(t_{ij}) = -V_{L+1}(1 - x_{L+1}) + \min_{1 \le j \le L}\left\{\frac{V_{L+1}}{m}\left(my_{L+1} + y'_j - \frac{S_{\max} + ms}{x_{L+1}}\right) + \frac{1}{2}U_1\omega_1\sum_{k=1}^{L} h(y_j,y_k,z_k)\right\}$$

where $S_{\max} = \max[0,y'_j - p(1 - x_{L+1})]$, $y'_j = \text{mod}(y_j - \delta_{L+1} - my_{L+1},p)$, $s = \max[0,x_{L+1} + y_{L+1} - 1]$, $z'_j = \text{mod}(z_j - my_{L+1},p)$ and $S_{\min} = \min[z'_j,px_{L+1}]$.

L-M System with Symmetric Delays

Intuitively, the tank size ought to be reduced by smoothening the input and output flow rates of the tank as much as possible. This can be achieved by spreading the starting moments of parallel units in a stage as far apart from each other as possible. In a stage with *L* parallel, identical units, the choice $y_i = (i - 1)/L$ accomplishes this. Operation with symmetric delays is of practical importance because of its simplicity. In the special *L*-1, batch/continuous case with identical units, Takamatsu et al. (1979) showed that the symmetric delay policy is in fact the optimum policy. Such a proof is not available in the general *L*-*M* case. However, our experiments with systems having identical units, indicate that symmetric delays in general yield the optimum storage capacity.

Consider an *L*-*M* system in which each stage consists of parallel, identical units and the units have the following fractional delay time values.

$$y_1 = 0$$
$$y_i = (i - 1)/L \qquad i = 1,L$$
$$y_i = y_{L+1} + (i - L - 1)/M \qquad i = L + 1,N$$
$$0 \le y_{L+1} < 1/M$$

The fractional delay time y_{L+1} can be visualized as the delay time of the downstream stage as a whole with respect to the upstream stage. This system is equivalent to a 1-1 system whose parameters and variables, identified by asterisks, are defined in Table 1.

For the *L*-*M* identical unit case (Takamatsu et al., 1979) have shown that the resultant input ($j = 1$) and output ($j = 2$) functions of the storage vessel can be expressed as:

$$F^*_j(t) = \begin{cases} c^*_j(\mu^*_j + 1)U^*_j & i\omega^*_j \le t \le (i + x^*_j)\omega^*_j \\ c^*_j\mu^*_jU^*_j & (i + x^*_j)\omega^*_j < t < (i + 1)\omega^*_j \end{cases} \quad j = 1,2$$

where $F^*_1(t) = \sum_{i=1}^{L} F_i(t - t_i)$; $F^*_2(t) = \sum_{i=L+1}^{N} F_i(t - t_i)$ and i is any integer. As a result, the holdup in the storage tank is described by

$$\frac{dV(t)}{dt} = \sum_{i=1}^{2} F^*_i(t - t^*_i) \qquad (16)$$

where $0 \le t^*_2 < \omega^*_2$ and $t^*_1 = 0$.

Notice that although the individual input functions have a cycle

TABLE 1. QUANTITIES FOR THE 1-1 SYSTEM EQUIVALENT TO *L*-*M* SYSTEM WITH IDENTICAL UNITS AND SYMMETRIC DELAYS

$U^*_1 = U_1, U^*_2 = U_N$	$z^*_i = \text{mod}(x^*_i + y^*_i,1)$
$\omega^*_1 = \omega_1/L, \omega^*_2 = \omega_N/M$	$c^*_1 = 1, c^*_2 = -1$
$x^*_1 = \text{mod}(Lx_1,1)$	$V^*_i = x^*_iU^*_i\omega^*_i, i = 1,2$
$x^*_2 = \text{mod}(Mx_N,1)$	$m^* = \omega^*_1/\omega^*_2$
$\mu^*_1 = \text{trunc}(Lx_1)$	$r = U^*_1/U^*_2$
$\mu^*_2 = \text{trunc}(Mx_N)$	$\beta^*_1 = L\beta_1/GCM(L\beta_1,M\beta_N)$
$t^*_1 = 0, t^*_2 = y_{L+1}\omega_N$	$\beta^*_2 = M\beta_N/GCM(L\beta_1,M\beta_N)$
$y^*_1 = 0, y^*_2 = My_{L+1}$	$p^* = 1/\beta^*_1$

TABLE 2. RESULTS FOR THE CALCULATIONS OF V_{max}, V_{min}, V^*

Range	Value	Expression
$r \geq 1$	V_{max}	$V_1^*(1 - x_1^*) + V_2^*\left[y_2^* - y_2^{*'} + \frac{S_{max} - s}{x_2^*}\right]$
		$S_{max} = \max[0, y_2^{*'} - p^*(1 - x_2^*)]$
	V_{min}	$-V_2^*(1 - x_2^*) + V_2^*\left[y_2^* - z_2^{*'} + \frac{S_{min} - s}{x_2^*}\right]$
		$S_{min} = \min[z_2^{*'}, p^* x_2^*]$
$r < 1$	V_{max}	$V_1^*(1 - x_1^*) - \frac{V_1^* y_2^{*'}}{m^*} + V_2^*\left[y_2^* + \frac{rS_{max} - s}{x_2^*}\right]$
		$S_{max} = \max[0, y_2^{*'} - p^*(1 - x_1^*)]$
	V_{min}	$-V_2^{*'}(1 - x_2^*) - \frac{V_1^* z_2^*}{m^*} + V_2^*\left[y_2^* + \frac{rS_{min} - s}{x_2^*}\right]$
		$S_{min} = \min[z_2^{*'}, p^* x_1^*]$

$y_2^{*'} = \mathrm{mod}(y_2^* - \delta_1^*, p^*)$, $z_2^{*'} = \mathrm{mod}(z_2^*, p^*)$, $s = \max[0, x_2^* + y_2^* - 1]$, $\delta_1^* = \mathrm{mod}(m^* x_1^*, p^*)$.

time of ω_1, their resultant input function has a cycle time of ω_1^* and the same holds true for the output functions. Moreover, the resultant input and output functions are composed of two parts. One part is the continuous one with flow rate $\mu_i^* U_i^*$ while the other is the batch part with flow rate U_i^*. Using this fact and representing $F_1^*(t)$ and $F_2^*(t)$ in terms of Fourier series, we have,

$$\frac{dV(t)}{dt} = \sum_{i=1}^{2} \sum_{n=1}^{\infty} \frac{2c_i^* U_i^*}{n\pi} \sin n\pi x_i^* \cos 2n\pi \left(\frac{t}{\omega_i^*} - \frac{x_i^*}{2}\right)$$

This equation is exactly identical to that of 1-1 system given by Karimi and Rekalitis (1983) and hence the aforementioned system is equivalent to a 1-1 system, characterized by quantities listed in Table 1. The analytical results, meant to be used for this system as well as any other 1-1 system are presented in Table 2.

Two implications of this equivalence to the 1-1 system are worth mentioning. First of all, the values $y_2^* = (1 - x_2^*)(1 - p^*)$ for $r \geq 1$ and $y_2^* = (1 - x_2^*) - p^*(1 - x_1^*)$ for $r < 1$ yield the minimum volume of the storage capacity. Second, the following ranges of y_2^* allow the operation of the system to be started with zero initial inventory.

$$(1 - x_2^*) - p^*(1 - x_2^*) \leq y_2^* \leq (1 - x_2^*) + p^* x_2^* \qquad r \geq 1$$
$$(1 - x_2^*) - p^*(1 - x_1^*) \leq y_2^* \leq (1 - x_2^*) \qquad r < 1$$

For a detailed discussion of 1-1 system, refer to the work by Karimi and Reklaitis (1983).

BOUNDS ON SIZE

We present here a method for obtaining a simple bound on the size. Since $V^* = V_{max} - V_{min}$, a bound can be easily obtained if one finds the maximum and the minimum values of V_{max} and V_{min}, respectively. We will be concerned only with the delay times as the variables and not the design variables such as cycle times, batch sizes, flow rates, etc., which will appear as parameters in the bounds.

The Fourier series expressions developed for holdup can be simplified to obtain an upper bound on V_{max} and a lower bound on V_{min}. The results are shown in the following proposition, the proof of which is given in Appendix II.

Proposition IV. For a general *L-M* system with one intermediate storage vessel,

$$\max_Y V_{max} < \sum_{i=1}^{L} U_i \omega_i h_{max}(i) - \sum_{i=L+1}^{N} U_i \omega_i h_{min}(i)$$
$$\min_Y V_{min} > \sum_{i=1}^{L} U_i \omega_i h_{min}(i) - \sum_{i=L+1}^{N} U_i \omega_i h_{max}(i)$$

and

$$\max_Y V^* < \sum_{i=1}^{N} V_i(1 - x_i)$$

where, $h_{max}(i) = z_i(y_i - z_i) + \max[0, z_i - y_i]$ and $h_{min}(i) = y_i(y_i - z_i) + \min[0, z_i - y_i]$.

An attractive feature of the bound given by Proposition IV is obviously its simplicity. The actual required size approaches the above bounds as g_i, $i = 1,N$ increase. In 1-1 system, this is equivalent to the increase in β_1. Physically, if the overall cycle time of the holdup is much larger than the individual cycle times of the two units in a 1-1 system, this bound serves as a very close estimate for the actual size.

SEARCH ALGORITHM

Unlike the 1-1 case, the analysis of the general *L-M* case does not readily yield direct expressions for the size of the storage vessel as a function of the Y vector. Consequently, to determine the optimal storage size and the correspondig Y vector, it is necessary to use a search algorithm. In this section, we present an algorithm based on a gradient method of minimax optimization for obtaining the optimum values of $V^*(Y)$.

Problem Formulation

The optimization problem is stated as follows:

$$P = \underset{Y}{\text{minimize}} \quad V^*(Y)$$
$$\text{subject to } \underline{y}_i \leq y_i \leq \bar{y}_i$$

From Eqs. 7 and 9, the Lemma III, it is clear that,

$$V^*(Y) = \max_{t^+ \epsilon T_{max}, t^- \epsilon T_{min}} [I(t^+, Y) - I(t^-, Y)]$$

Let $T_{max} \times T_{min}$ denote the set of ordererd pairs of the elements of T_{max} and T_{min} and let t_k^+ and t_k^- be the elements of the kth ordered pair, then

$$T_{max} \times T_{min} = [(t_k^+, t_k^-): t_k^+ \epsilon T_{max}; t_k^- \epsilon T_{min}; 1 \leq k \leq N_T]$$

where, $N_T = [\sum_{j=1}^{N} \beta_j]^2$. Furthermore, define $H_k(Y)$ *as*,

$$H_k(Y) = I(t_k^+, Y) - I(t_k^-, Y) \qquad (17)$$

Clearly, $V^*(Y) = \max_{1 \leq k \leq N_T} H_k(Y)$. Hence,

$$P = \min_Y \max_{1 \leq k \leq N_T} H_k(Y)$$

is a discrete minimax problem. Most of the work on the solutions of minimax problems has been centered on problems in continuously differentiable functions. One of the approaches to the solution of such problems is the use of gradient information of one or more of the functions to obtain a downhill direction by solving a suitable linear programming problem (Bandler et al., 1972). In our case, however, the functions $H_k(Y)$ are not continuously differentiable but are piecewise linear with respect to individual variables. Hence, our approach is to use two-sided (left hand side and righthand side) partial derivatives and then construct a downhill gradient direction without solving a linear program. As all the functions involved are piecewise linear, our solution methodology is successful, though not mathematically rigorous. First of all, we note the following proposition about the nature of functions $H_k(Y)$.

Proposition V. The functions $H_k(Y)$ are continuous.

As evident from the following lemma (Dem'yanov and Malozemov, 1974) which we state without proof, the above proposition has a very important consequence.

Lemma IV. If all the functions $H_k(Y)$, $1 \leq k \leq N_T$ are continuous at a point Y_0, $V^*(Y)$ is also continuous at Y_0.

Fixing Y, let us consider the set of indices $R(Y)$ defined by

$$R(Y) = [k: 1 \leq k \leq N_T; H_k(Y) = V^*(Y)] \qquad (18)$$

The following lemma (Dem'yanov and Malozemov, 1974) ensures that the set $R(Y_0 + \gamma d)$ is a subset of $R(Y_0)$ for local variations around Y_0 in the direction d.

Lemma V. If the functions $H_k(Y)$, $1 \le k \le N_T$ are continuous at a point Y_0, there exists a number $\gamma_0 > 0$ such that $\forall\ \gamma \epsilon [0,\gamma_0]$ and $d \epsilon E_N$, $\|d\| = 1$,

$$V^*(Y_0 + \gamma d) = \max_{k \epsilon R(Y_0)} [H_k(Y_0)] \qquad (19)$$

On the basis of above results, we can evaluate two-sided partial derivatives of $V^*(Y)$ and then use the resultant direction as the direction for a linear search. After finding an optimum along this direction, implicitly taking care of the bounds on Y, we repeat the procedure. The search is terminated when no further decrease in $V^*(Y)$ can be found.

The key step in the procedure involves the calculation of the partial derivatives of $V^*(Y)$. To obtain these, we first need those of the function $I(t)$.

Proposition VI. For $I(t)$ as defined by Eq. 7.

$$\left.\frac{\partial I(t)}{\partial y_j}\right|_{t \text{ fixed}} = \omega_i [F_j(-t_j) - F_j(t - t_j)] \qquad j > 1$$

$$\left.\frac{\partial I(t)}{\partial y_j}\right|_{(t-t_j) \text{ fixed}} = \omega_j [\sum_{i=1,j}^{N} F_i(t - t_i) + F_j(-t_j)] \qquad j > 1$$

Notice that any $t \epsilon T$ can be represented as $t = t_j + a_{ij}$, where a_{ij} is a constant. If we analyze the behavior of $I(t)$ with respect to y_k, $k \ne j$, t is fixed and we use the first derivative from Proposition VI. On the other hand, if y_j itself is the variable, it is $t - t_j$ which is constant and hence, we use the second derivative from Proposition VI. From Eq. 19, we have,

$$\frac{\partial V^*(Y)}{\partial y_j} = \max_{k \epsilon R(Y)} \frac{\partial H_k(Y)}{\partial y_j}$$

Furthermore, from Eq. 17 and the above result, we get,

$$\left.\frac{\partial V^*(Y)}{\partial y_j}\right|_{y_j+0} = \max_{k \epsilon R(Y)} \left.\frac{\partial I(t_k^+,Y)}{\partial y_j}\right|_{y_j+0} - \min_{k \epsilon R(Y)} \left.\frac{\partial I(t_k^-,Y)}{\partial y_j}\right|_{y_j+0}$$

$$\left.\frac{\partial V^*(Y)}{\partial y_j}\right|_{y_j-0} = \max_{k \epsilon R(Y)} \left.\frac{\partial I(t_k^+,Y)}{\partial y_j}\right|_{y_j-0} - \min_{k \epsilon R(Y)} \left.\frac{\partial I(t_k^-,Y)}{\partial y_j}\right|_{y_j-0}$$

Clearly, the jth element of the search direction vector d is given by,

$$d_j = 0 \text{ if } \min \left[\left.\frac{\partial V^*}{\partial y_j}\right|_{y_j+0}, \left. -\frac{\partial V^*}{\partial y_j}\right|_{y_j-0}\right] \ge 0$$

or

$$d_j = -\left.\frac{\partial V^*}{\partial y_j}\right|_{y_j-0} \text{ if } \left.\frac{\partial V^*}{\partial y_j}\right|_{y_j+0} + \left.\frac{\partial V^*}{\partial y_j}\right|_{y_j-0} > 0$$

or

$$= -\left.\frac{\partial V^*}{\partial y_j}\right|_{y_j+0}$$

Description of Algorithm

The algorithm starts with an initial estimate of the fractional delay time vector Y_0. The function $V^*(Y_0)$ is determined by the general procedure for sizing. The formulation for the general sizing procedure facilitates the determination of $R(Y_0)$ and the derivatives of $I(t_k^+)$ and $I(t_k^-)$ for $k \epsilon R(Y_0)$. This is true since, as shown in Proposition VI, the derivatives of $I(t)$ very much depend on the unit whose delay time is varying. The general sizing procedure readily identifies t_k^+ and t_k^-, $k \epsilon R(Y_0)$ with units whose events they represent. After the evaluation of the partial derivatives of $V^*(Y)$, the search direction d is obtained as shown above. The optimum step parameter γ is determined by performing a line search along the direction d such that $0 \le \gamma \le \gamma_{\max}$, where $\gamma_{\max}$ is suitably calculated to keep the y_i values within the bounds. The y_i values can be further adjusted by using Theorem I, thus $\gamma_{\max} > 0$ can always be satisfied whenever any of the y_i values hits the bound and can not be changed further along the direction d. This procedure is repeated starting with the new optimum point found along the direction d. The search terminates when d is the zero direction.

Performance Evaluation

The function $V^*(Y)$ is multimodal in Y and hence determination of the global solution requires the use of a restart strategy. Specifically, the gradient method outlined above must be restarted from a number of different initial estimates and the best of the local optima selected as the global solution. In addition, because of the discontinuous derivatives of the maximum function, convergence to a stationary point is not guaranteed with gradient methods for minimax optimization. The initial estimates of Y should be such that y_i values are spread out uniformly over the feasible range, as defined by Theorem I. Of course, the problem could also be solved using direct search methods as noted by Oi et al. (1977) and Takamatsu et al. (1979). To test the effectiveness of our gradient approach, Powell's conjugate directions procedure was modified to implicitly handle bounds on the variables and a number of tests were run using both methods.

Sample results from a set of 79 test problems are summarized in Table 3. Overall, the gradient procedure is slower than the direct search in only nine cases, terminates faster but with a worse local solution in 36 cases, and terminates faster with the same or better solution in the remaining 34 cases. In general, the gradient direction is quite effective as indicated by the generally much lower number

TABLE 3. COMPARISON BETWEEN PCD METHOD AND GRADIENT METHOD

			PCD Results				GRD Results			
No.	System	Initial V^*	Final V^*	CPU Time (s)	Line Searches	Function Count	Final V^*	CPU Time (s)	Line Searches	Function Count
1	1-2	1.736	1.179	0.94	10	109	1.350	0.23	1	26
2	1-2	2.000	1.371	0.84	6	78	1.371	0.34	1	27
3	1-3	4.000	3.900	6.45	6	32	4.000	0.30	0	1
4	1-4	2.571	2.439	2.73	13	107	2.419	0.68	1	28
5	1-4	4.292	3.792	10.12	40	360	3.792	2.50	10	84
6	1-5	4.520	2.360	4.57	21	131	2.360	2.09	5	56
7	1-5	0.702	0.347	27.06	46	3140	0.311	0.35	1	29
8	1-5	2.889	1.836	25.47	37	561	2.500	0.72	3	13
9	2-1	1.500	1.000	0.35	4	28	1.000	0.16	1	9
10	2-2	2.867	2.800	7.21	6	35	2.800	1.95	1	9
11	2-2	3.050	2.790	18.64	9	90	2.915	2.14	1	10
12	2-3	5.596	4.946	12.52	8	83	5.241	5.90	3	39
13	3-1	4.400	3.000	1.27	6	50	3.133	1.83	3	70
14	3-1	2.050	1.500	4.10	13	161	1.844	0.40	1	11
15	3-2	5.525	4.200	43.43	12	108	4.238	32.12	3	79
16	4-1	4.667	4.250	6.84	17	180	4.250	0.41	1	8
17	4-1	3.063	1.700	5.28	12	85	1.900	0.98	1	15
18	5-1	1.500	1.050	43.45	84	834	1.300	1.91	2	34
19	5-1	1.600	0.560	3.52	10	80	1.500	0.41	1	7
20	5-1	0.775	0.600	2.80	8	77	0.600	1.93	2	49

TABLE 4. DATA FOR THE EXAMPLE

Unit No.	V kg	T_s h	T_i h	T_f h	T_e h	T_B h	T_p h	t h
1	900	—	—	0.75	0.75	4.5	4.5	0.0
2	2,250	—	—	1.50	1.50	6.0	0.0	4.5
3	1,500	9	10	—	—	—	—	0.0
4	1,000	6	2	—	—	—	—	0.0
5	500	3	1	—	—	—	—	0.0

TABLE 5. PARAMETERS FOR THE EXAMPLE

Unit No.	ω h	β	x	U kg/h	y	z
1	6	60	.125	1200	0.0	.125
2	9	40	.167	1500	0.5	.667
3	10	36	.900	166.67	0.0	.900
4	8	45	.750	166.67	0.0	.750
5	4	90	.750	166.67	0.0	.750

of line searches required by the gradient algorithm and the large proportion of cases (31 of 79) in which the local optimum is found in a single-line search. In general, with either search method, restarts are required to identify the global optimum hence speed of the search is of considerable interest. Speed is also of concern since the above optimal volume determination is likely to be performed as a subproblem solution within an overall scheme for batch/semicontinuous process design (Takamatsu et al., 1982).

EXAMPLE

An intermediate storage vessel acts as a surge between an upstream stage with two batch units and a downstream stage with three semicontinuous units. Calculate the limiting size of the storage tank and an upper bound on the same. Also, find the period of the storage size with respect to the individual delay times. The parameters of the units are given in Table 4.

By direct appliction of the appropriate definitions to the data of Table 4, we obtain the quantities listed in Table 5. Note that the productivities of both stages are equal to 400 kg/h so assumption 3 of our model is satisfied.

The 2-3 system consists of nonidentical units and hence we must employ the sizing procedure for a general system. As is evident from Lemma III for V_{max}, we need to calculate $I(t_{ij})$ at the following values of t_{ij},

$$t_{i1} = 0.75 + 6i \qquad 0 \le i < 60$$

$$t_{i2} = 6 + 9i \qquad 0 \le i < 40$$

$$t_{i3} = 10i \qquad 0 \le i < 36$$

$$t_{i4} = 8i \qquad 0 \le i < 45$$

$$t_{i5} = 4i \qquad 0 \le i < 90$$

while V_{min} can be obtained by calculating $I(t_{ij})$ at the following values of t_{ij},

$$t_{i1} = 6i \qquad 0 \le i < 60$$

$$t_{i2} = 4.5 + 9i \qquad 0 \le i < 40$$

$$t_{i3} = 9 + 10i \qquad 0 \le i < 36$$

$$t_{i4} = 6 + 8i \qquad 0 \le i < 45$$

$$t_{i5} = 3 + 4i \qquad 0 \le i < 90$$

Using the result of Proposition II, $I(t)$ must be calculated at these 542 points, then V_{max} and V_{min} are determined by comparison to obtain $V_{max} = 1{,}275$ kg and $V_{min} = -1{,}333.3$ kg. Hence, the size of the storage vessel must be 2,608.3 kg and an initial inventory of 1,333.3 kg is required in the storage tank so that the storage vessel neither runs out of material at the time of demand by the semicontinuous units nor overflows.

An upper bound on the limiting size of the tank is easily calculated with the help of Proposition IV to be 3,187.5 kg. The bounds on the values of V_{max} and V_{min} for this set of delay times were obtained as $V_{max} < 1{,}537.5$ kg and $V_{min} > -1{,}650$ kg. From Theorem I, we obtain $g_1 = 1$, $g_2 = 3$, $g_3 = 5$, $g_4 = 2$ and $g_5 = 1$. Hence, the tank size is periodic with respect to individual fractional delay times having periods of 1, 1/3, 0.2, 0.5 and 1, respectively. Therefore, the typical ranges of y_i's which include all possible values of $V^*(Y)$ are: $y_1 = 0$, $0 \le y_2 \le 1/3$, $0 \le y_3 < 0.2$, $0 \le y_4 \le 0.5$, $0 \le y_5 < 1$. For example, $Y = (0, 0.5, 0, 0, 0)$, $Y = (0, 1/6, 0.2, 0.5, 0)$, $Y = (0.5/6, 0.6, 0.5, 0)$ etc. result in the same V^* but different V_{max} and V_{min}.

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NOTATION

a_{ij}	= a constant derived from the cycle times and delay times of unit i and j
c	= a coefficient assigned to every unit
d	= search direction vector ($N \times 1$)
E_N	= N-dimensional euclidean space
$f(t)$	= general flow rate function for a unit
$F(t)$	= characteristic flow function for a unit
g	= GCM as defined in Theorem I
h	= function defined in Proposition II
h_{max}	= function defined in Proposition IV
h_{min}	= function defined by Proposition IV
$H(Y)$	= function defined in Eq. 17
$I(t)$	= function defined in Eq. 7
L	= number of units in the upstream stage
m	= ratio of cycle times defined for Proposition IIa and IIb
M	= number of units in the downstream stage
N	= total number of units, $L + M$
N_T	= total number of H functions
P	= defined as $1/\beta_1$ for Proposition IIa and $1/\beta_{L+1}$ for Proposition IIIb
p^*	= defined in Table 1
r	= defined as U_1^*/U_2^*
R	= a set of indices defined by Eq. 18
t	= time
t^+	= an element of set T_{max}
t^-	= an element of set T_{min}
t_k^+, t_k^-	= elements of the ordered pair (t_k^+, t_k^-) in the set $T_{max} \times T_{min}$
t_i	= delay time for unit i
T	= set of all the corner points of the holdup function
T_e	= time required to empty a batch unit
T_f	= time required to fill a batch unit
T_i	= shutdown time for a semicontinuous unit
T_{max}	= set of candidates $t_{ij}, t_{ij} \epsilon T$ for $I(t_{ij}) = V_{max}$
T'_{max}	= a subset of T_{max} defined for systems with identical units
T_{min}	= set of candidates $t_{ij}, t_{ij} \epsilon T$ for $I(t_{ij}) = V_{min}$
T'_{min}	= a subset of T_{min} defined for systems with identical units
T_p	= preparation time and waiting time for a batch unit
T_B	= processing time of a batch unit
T_S	= processing time for a semicontinuous unit
u	= a variable defined in Eq. 13
U	= constant input or output flow rate of a unit
V	= batch size of a unit
$V(t)$	= holdup in the storage vessel
V_{max}	= maximum value of $I(t)$
V_{min}	= minimum value of $I(t)$
V^*	= limiting size required to decouple the upstream and

downstream stage

x = characteristic fraction for a unit as defined in Eq. 1

y = fractional delay time variable of a unit as defined in Eq. 4

$\underline{y}$ = lower bound on y

$\bar{y}$ = upper bound on y

Y = N-dimensional vector of fractional delay times $(y_1, y_2, \ldots, y_N)$

z = $\mathrm{mod}(x + y, 1)$ as in Eq. 12

Greek Letters

α = integer variable

β = characteristic integer of a unit defined as Ω/ω

γ = step size in the search direction d

γ_{max} = maximum value of step size satisfying the bounds on Y

ω = cycle time of a unit

Ω = least common multiple of $\omega_1, \omega_2, \ldots, \omega_N$

δ_i = $\mathrm{mod}(mx_i, p)$

τ, θ = dummy variables

Subscripts and Superscripts

i, j = units i, j

* = quantities for the 1-1 system equivalent to an L-M system with symmetric delay times

Mathematical Symbols

$GCM(\ )$ = greatest common measure of the quantities within the parenthesis

$LCM(\ )$ = least common multiple of the quantities within the parenthesis

max[ ] = maximum of the quantities within the bracket

min[ ] = minimum of the quantities within the bracket

$\mathrm{mod}(x,y)$ = z such that $x = ky + z$ for some integer k and $0 \le z < y$

$sgn(x)$ = $x/|x|$

trunc(x) = the greatest integer in x

$|\ |$ = absolute value

$[x]_+$ = x if $x \ge 0$ and 0 if $x < 0$

APPENDIX I: PROOF OF THEOREM I

Let $a_{ni}, n = 0,\infty$ and $b_{ni}, n = 1,\infty$ be the Fourier series coefficients for $f_i(t)$. Since, $a_{0i} = V_i/\omega_i$, we have,

$$\frac{dV(t)}{dt} = \sum_{i=1}^{N}\sum_{n=1}^{\infty} c_i\left[a_{ni}\sin 2n\pi\left(\frac{t}{\omega_i} - y_i\right) + b_{ni}\cos 2n\pi\left(\frac{t}{\omega_i} - y_i\right)\right]$$

Let $G(v,w) = I(v) - I(w)$, where $I(t) = V(t) - V(0)$ as defined earlier and v and w are any two instances of time. Integrating the above differential equation term by term, we obtain,

$$G(v,w) = \sum_{i=1}^{N}\sum_{n=1}^{\infty}\left\{-A_{ni}\left[\cos 2n\pi\left(\frac{v}{\omega_i} - y_i\right) - \cos 2n\pi\left(\frac{w}{\omega_i} - y_i\right)\right] + B_{ni}\left[\sin 2n\pi\left(\frac{v}{\omega_i} - y_i\right) - \sin 2n\pi\left(\frac{w}{\omega_i} - y_i\right)\right]\right\}$$

where for simplicity the coefficients, A_{ni} and B_{ni} include the original coefficients as well as those resulting from the integration.

Now $v = \alpha\omega_1 + v'\omega_1$, $0 \le v' < 1$, α integer and $w = \beta\omega_1 + w'\omega_1$, $0 \le w' < 1$, β integer, hence,

$$G(\alpha,\beta,y,v_i,w_i) = \sum_{i=1}^{N}\sum_{n=1}^{\infty}\left\{\beta_{ni}\left[\sin 2n\pi\left(\frac{\alpha\beta_i}{\beta_1} + v_i - y_i\right) - \sin 2n\pi\left(\frac{\beta\beta_i}{\beta_1} + w_i - y_i\right)\right] - A_{ni}\left[\cos 2n\pi\left(\frac{\alpha\beta_i}{\beta_1} + v_i - y_i\right) - \cos 2n\pi\left(\frac{\beta\beta_i}{\beta_1} + w_i - y_i\right)\right]\right\}$$

For fixed values of

$$v_i = \frac{v'\omega_1}{\omega_i},\ w_i = \frac{w'\omega_1}{\omega_i}$$

and $y_i, i \neq j$, we have $G(\alpha,\beta,y,v_i,w_i) \equiv g(\alpha,\beta,y_j)$. Note that $\beta_i, i = 1,N$ are the least integers, hence, $GCM(\beta_1,\beta_2,\ldots,\beta_N) = 1$ and $GCM(g_j,\beta_j) = 1$. Furthermore, there exists an integer q_i, such that $\beta_i = q_i g_j$, $\forall i \neq j$.

Lemma A1. If $GCM(a,n) = 1$, there exists an integer x, $0 < x < n$ such that $\mathrm{mod}(ax,n) = n - 1$ (Dorothy, 1982).

Proof. First, we will prove that if $GCM(a,n) = 1$, $\mathrm{mod}(ai,n) \neq \mathrm{mod}(aj,n)$ for each i,j such that $0 \le i < j < n$. Let us assume the contrary. Then n divides $a(i-j)$. Since $GCM(a,n) = 1$, $(i-j)$ must be a multiple of n, which is impossible as both i and j are smaller than n. This property implies that each $\mathrm{mod}(ai,n)$, $i = 0,\ldots,n$-1, is a distinct residue and the set $\{r_i : r_i = \mathrm{mod}(ai,n), 0 \le i < n\}$ is a permutation of the complete set of residues $[0,1,2,\ldots,n\text{-}1]$. Therefore, $x = i$, where $\mathrm{mod}(ai,n) = n\ 1$ is the required integer.

From the above Lemma, there exists an integer n^* such that $\mathrm{mod}(\beta_j n^*, g_j) = g_j - 1$ for $0 \le n^* < g_j - 1$. Now, one can easily verify that

$$G(\alpha,\beta,y_j + 1/g_j) = G(\alpha + n^*q_1, \beta + n^*q_1, y_j)$$

Therefore, given two arbitrary points $t = v$ and $t = w$ in the profile of $I(t)$ for $y_j + 1/g_j$, one can always find two points $t = (\alpha + n^*q_1)\omega_1 + v'\omega_1$ and $t = (\beta + n^*q_1)\omega_1 + w'\omega_1$ in the profile of $I(t)$ for y_j such that function G has the same value in both cases. Notice that our choice for v and w was arbitrary and hence the above statement is valid for all pairs of v and w. But, $V^* = \max_{v,w} G(v,w)$ and hence, $V^*(y_j)$ is a periodic function with respect to y_j with period $1/g_j$.

APPENDIX II: PROOF OF PROPOSITION IV

From the definition of $h(u_i,y_i,z_i)$ in Proposition II, $\lim_{u_i \to 1} [h(u_i,y_i,z_i)] = 0$ and $h(0,y_i,z_i) = 0$. Rearranging $h(u_i,y_i,z_i)$, we get,

$$h(u_i,y_i,z_i) = 2u_i(y_i - z_i) + [2sgn(z_i - y_i)]\{[u_i - \min(y_i,z_i)]_+ - [u_i - \max(y_i,z_i)]_+\}$$

First, we consider the case of $y_i \le z_i$. Clearly, $h(u_i,y_i,z_i) = 2u_i(y_i - z_i) + 2[u_i - y_i]_+ - 2[u_i - z_i]_+$. Now, $h(y_i,y_i,z_i) = 2y_i(y_i - z_i)$ and $h(z_i,y_i,z_i) = 2(1 - z_i)(z_i - y_i)$. Moreover, one can verify that $h(u_i,y_i,z_i) - h(y_i,y_i,z_i) \ge 0$ and $h(u_i,y_i,z_i) - h(z_i,y_i,z_i) \le 0$ for $0 \le u_i < 1$ and hence,

$$\max_{u_i} h(u_i,y_i,z_i) = 2(1 - z_i)(z_i - y_i) \text{ and } \min_{u_i} h(u_i,y_i,z_i) = 2y_i(y_i - z_i)$$

Similar treatment for $y_i > z_i$ yields,

$$\max_{u_i} h(u_i,y_i,z_i) = 2z_i(y_i - z_i) \text{ and } \min_{u_i} h(u_i,y_i,z_i) = 2(1 - y_i)(z_i - y_i)$$

Combining the above results with the results of Proposition II and defining $h_{max}(i) = \max_{u_i} 1/2\, h(u_i,y_i,z_i)$ and $h_{min}(i) = \min_{u_i} 1/2\, h(u_i,y_i,z_i)$ the results of Proposition IV follow.

APPENDIX III: PROOF OF PROPOSITION V

It suffices to prove that $I(t,Y)$ is a continuous function of Y for

$t \epsilon T$. Let E_N denote the euclidean N-space whose elements are vectors $Y = (y_1, y_2, \ldots, y_N)$. Note that any $t \epsilon T$ can be represented as $t = a_j + y_j \omega_j$ for some 1, $1 \leq j \leq N$. Clearly,

$$I(t,Y) = \sum_{i=1}^{N} I_i(Y) \qquad \text{where, } I_i(Y) = \int_{-y_i\omega_i}^{a_1 + y_j\omega_j - y_i\omega_i} F_i(\tau) d\tau$$

Let $Y_0 \epsilon E_N$. As $I_i(Y)$ is continuous with respect to y_j and y_i separately, for a given $\epsilon' = \epsilon/2N > 0$, there exists a $\delta > 0$ such that $|I_i(Y) - I_i(Y_0)| < \epsilon/N$ and hence, $|I(t(y_j),y) - I(t(y_{0j});y_0)| < \epsilon$ for $||y - y_0|| < \delta$.

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Hydrodynamic Parameters for Gas-Liquid Cocurrent Flow in Packed Beds

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The hydrodynamics of cocurrent gas-liquid flow in packed beds is analyzed by extending the concept of relative permeability to the inertial regime.

The relative permeabilities of the gas and liquid phases are functions of the saturation of the liquid phase. These functions are found from an analysis of experimental data. The relations obtained are used to develop empirical correlations for predicting liquid holdup and pressure drop in gas-liquid cocurrent downflow in packed beds over a wide range of operating conditions. The correlations proposed give very good results when compared to experimental data yielding, in general, mean relative deviations lower than existing correlations. In addition, a new equation is proposed for predicting static holdup in packed beds which is based on a more physically realistic characteristic length than that used in previous studies.

SCOPE

The prediction of the liquid holdup and pressure drop for two-phase flow in packed beds is of great importance in industrial processes. This kind of problem presents itself in a wide variety of applications, such as in trickle-bed reactors and packed-bed gas-liquid absorbers. The study of flow regimes, pressure drop and holdup in these systems has been conventionally treated from a completely empirical point of view due to the complexity of the problem. This has induced the development of a large diversity of methods of analysis in the literature; as a result, there now exist several different empirical correlations for predicting these hydrodynamic parameters.

The objective of this work is to provide a rational approach to predict pressure drops and liquid holdups for the case of gas-liquid cocurrent down-flow through packed beds and to develop new correlations to estimate those hydrodynamic parameters.

The analysis presented in this work is based on the use of the traditional concepts of capillary pressure and relative permeabilities to model the hydrodynamics of two-phase flow in packed beds. One of the main goals of this study is to determine how the gas and liquid relative permeabilities for both the viscous and inertial flow regimes are affected by the operating conditions, the structure of the medium, and the physical properties of the fluids.

CONCLUSIONS AND SIGNIFICANCE

A semiempirical approach is used to analyze the hydrodynamics of cocurrent gas-liquid flow in packed beds.

A correlation for predicting static holdup is presented (Eq. 8). It is a simple modification of the existent correlation of Charpentier et al. (1968); even though it does not improve considerably the accuracy of the prediction, it is based on a

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