A Single Particle Approach for Analyzing Flow Systems

Part III: Multiple Fluids

This paper provides a stochastic model for general flow systems with several inlets and outlets, where different fluids are fed through the various inlets. Several process characteristics are derived and discussed. They include the distribution, mean, and variance of the number of visits and total residence time of the various fluid elements to flow regions and the fraction of each fluid that avoids a flow region or a group of flow regions. It is shown that for any fluid and any specified region, the local flow rate through the region is equal to the product of the net flow rate through the system and the mean number of visits to the region by a fluid element of this type. Expressions are also derived for the compositions of material at the outlet streams and at individual flow regions exits, as well as for the composition of material inside each flow region. These results may be employed to verify flow models of physical systems and to determine model parameters.

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SCOPE

In Parts I and II of this series (Rubinovitch and Mann, 1983a,b) a stochastic methodology for analyzing chemical engineering systems was developed. This methodology is based on considering the history of individual fluid elements (or particles) as they pass through the system. Some new results were obtained, and computational methods were described relating to the number of visits by a particle to a flow region or group of flow regions. Further, a basic relation that ties together local flow rates and number of visits to a region was obtained. The potential applications of this relationship were recently discussed (Mann and Rubinovitch, 1983). In this paper the analysis is extended to systems with several inlets and several outlets where different types of fluid elements are fed through the various inlets.

CONCLUSIONS AND SIGNIFICANCE

This paper provides results and computational methods regarding a variety of system characteristics that are of interest in multifluid (or multiparticle) flow systems at steady state. The results include a fundamental relationship tying together local bulk properties (flow rates) with individual particle behavior (number of visits to a region). It says that for each fluid type and for any given fixed local zone (region),

$$\begin{pmatrix}\text{Local flow rate}\\ \text{through the region}\end{pmatrix} = \begin{pmatrix}\text{Net flow rate}\\ \text{through the system}\end{pmatrix} \times \begin{pmatrix}\text{Mean number of}\\ \text{visits to the region}\\ \text{by a fluid element}\end{pmatrix}$$

In other words, local flow rates are proportional to the flow rate through the system, and the proportionality coefficient is the mean number of visits to the region. This relationship also holds true for aggregates of several fluids and for aggregates of several regions.

The method of proving this result is probabilistic, and the key parameter, the number of visits to a region, is a probabilistic concept new in chemical engineering. The derivation of this basic relationship demonstrates the important role that probability theory could play in chemical engineering.

This paper also provides expressions for other systems' characteristics related to the concepts of number of visits to a region and to total regional residence times. In particular, this basic relationship provides a link between the overall material composition inside a region, the composition of material at the region's outlet (or inlet), and the mean sojourn times of the individual fluid types. The relationship indicates a potential experimental method for determining local sojourn times and for verifying model parameters.

Parts I and II of this series appeared in *AIChE J.*, 29, 658 and 663 (1983).

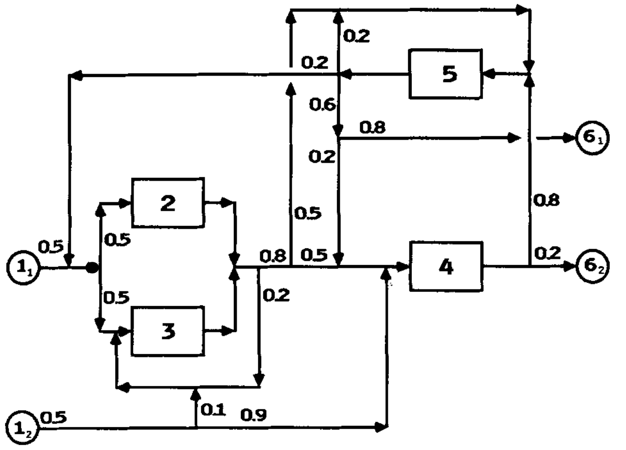

Figure 1. Schematic description of a system with multiple inlets and outlets.

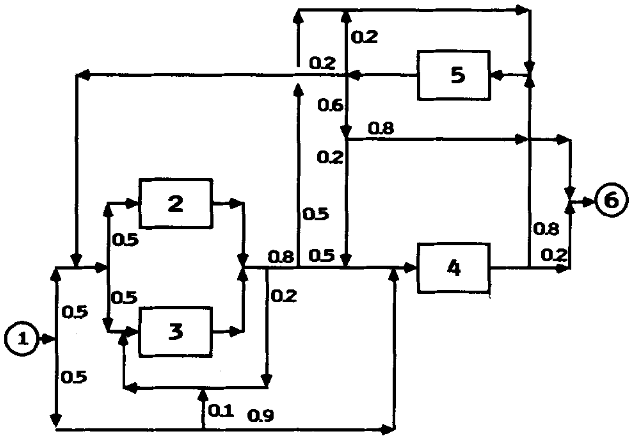

Figure 2. The system of Figure 1 applied to a single fluid.

INTRODUCTION

This paper is a continuation of Part I and Part II (Rubinovitch and Mann, 1983a,b), presenting a methodology for characterizing and analyzing general chemical engineering flow processes with special emphasis on particulate processes. Here the analysis is extended to systems with several inlets, several outlets, and more than one type of fluid. The system may be any flow system or flow model at steady state with several flow regions that are interconnected in a specified yet arbitrary way. There were no restrictions on the structure of the system or on internal mixing or flow patterns.

If there is only one type of fluid in the system, then one is usually interested in the same system characteristics as those studied in Parts I and II, and these can be derived using the methods described there. All one has to do is combine all inlets into one new (fictitious) inlet and all outlets into one (fictitious) outlet. As an illustration, consider the flow diagram of Figure 1 and assume that each inlet feeds into the system 50% of the entering material. When we combine the inlets and the outlets, respectively, we obtain the system shown in Figure 2.

The matrix of transition probabilities for this new system is

$$\bar{P} = \begin{bmatrix} 0 & 0.25 & 0.30 & 0.45 & 0 & 0 \\ 0 & 0 & 0.2 & 0.4 & 0.4 & 0 \\ 0 & 0 & 0.2 & 0.4 & 0.4 & 0 \\ 0 & 0 & 0 & 0 & 0.8 & 0.2 \\ 0 & 0.1 & 0.1 & 0.12 & 0.2 & 0.48 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

and all the characteristics studied in Parts I and II can be derived in exactly the same way as before.

The situation is quite different in the more general case when different types of fluids enter the system through the different inlets. This is of course the case in most operations. In what follows we extend the methods of Parts I and II to multiparticle systems and introduce new characteristics of importance in such systems.

MULTIPARTICLE SYSTEMS: VISITS TO FLOW REGIONS

Consider a general flow system, or model, with several flow regions and with several inlets and outlets. Each inlet is feeding the system with a different type of fluid. For the time being we assume that each region has one inlet and one outlet, but the system has several inlets and outlets. Also, we assume that the system is in steady state and the particles do not change in the system (e.g., by chemical reaction).

Let us say that the system has l inlets labeled $1_1,\ldots,1_l$, $r-1$ flow regions, labeled $2,3,\ldots,r$, and s outlets labeled $0_1,\ldots,0_s$. Fluid elements that enter the system through inlet 1_1 will be called type 1 particles, those entering the system through inlet 1_2 will be called type 2 particles, etc. To begin with, assume that all particles obey the same laws of movement in the system. An example of such a system with two inlets, four flow regions, and two outlets is shown in Figure 1.

Let $X_n (n \geq 1)$ be the number of the nth flow region that a particle visits and, let X_o be the inlet through which it enters the system. The process $X = \{X_n : n = 0,1,2,\ldots\}$ is a Markov chain with stationary transition probabilities and finite state space. The inlets and all flow regions are transient states, and the outlets are absorbing states. (See, for example, Çinlar [1975] for the meanings of these terms.) As before, we shall write $\bar{P} = \{P(i,j)\}$ for the matrix of transition probabilities, which, for the example of Figure 1, is

$$\bar{P} = \begin{bmatrix} 0 & 0 & 0.5 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.1 & 0.9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.2 & 0.4 & 0.4 & 0 & 0 \\ 0 & 0 & 0 & 0.2 & 0.4 & 0.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.8 & 0 & 0.2 \\ 0 & 0 & 0.1 & 0.1 & 0.12 & 0.2 & 0.48 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Here, the first two rows and columns correspond to inlets 1_1 and 1_2, the next four rows and columns correspond to flow regions 2, 3, 4, and 5, and the last two rows and columns to the two outlets 0_1 and 0_2.

Suppose now that the fraction of particles entering the system through inlet 1_1 is $\pi(1)$, through inlet 1_2 is $\pi(2)$, etc., and that the flow rates through the respective inlets (particles per unit time) are $w_o(1),\ldots,w_o(l)$. Then

$$\pi(i) = w_o(i) / \sum_{1}^{l} w_o(i).$$

The vector $\bar{\pi} = (\pi(1),\ldots,\pi(l))$ is the initial distribution of the Markov chain X, and must satisfy $\pi(i) \geq o$ for $1 \leq i \leq l$ and $\Sigma\pi(i) = 1$. The number $\pi(i)$ is the probability that a randomly chosen particle that enters the system is of type i, i.e., $\pi(i) = P\{X_o = 1_i\}$. The matrix $\bar{P}$ and the vector $\bar{\pi}$ completely determine the Markov chain X.

With this we proceed, as in Part I, to define the random variable N_j (the number of visits to region j), the matrix $R = \{R(i,j)\}$, and the numbers $F(i,j)$. Again, $\bar{R}(i,j) = E[N_j | X_o = 1_i]$ is the mean number of visits to region j by a type i particle, and $F(i,j)$ is the probability that a type i particle will ever enter region j.

The computation of $R(i,j)$ for $i = 1_1,\ldots,1_l,2,\ldots,r$ and $j = 2,\ldots,r$ is exactly as in Part I using

$$\overline{R} = (\overline{I} - \overline{Q})^{-1} \qquad (1)$$

where I is the identity matrix and $\overline{Q}$ is the matrix obtained from $\overline{P}$ by deleting all rows and columns that correspond to the outlets (see also Eqs. 10 and 11 in Part I). The distribution of the number of visits to region j by a type i particle is

$$P_{1_i}(N_j = m) = \begin{cases} 1 - p_j(i) & m = 0 \\ p_j(i) q_j^{m-1}(1 - q_j) & m = 2,\ldots,r \end{cases} \qquad (2)$$

where $q_j = F(j,j)$ is the probability that a particle leaving region j will ever return to this region and

$$p_j(i) = F(1_i,j) \qquad (3)$$

is the probability that a type i particle visits region j at least once. The mean and variance of the number of visits to region j by type i particles are

$$E_{1_i}[N_j] = R(1_i,j) \qquad (4)$$

$$\mathrm{Var}_{1_i}[N_j] = \frac{p_j(i)(1 + q_j - p_j(i))}{(1 - q_j)^2} \qquad (5)$$

For the example of Figure 1 using Eqs. 10, 11, and 20 of Part I, we find that

$$\overline{Q} = \begin{bmatrix} 0 & 0 & 0.5 & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0.1 & 0.9 & 0 \\ 0 & 0 & 0 & 0.2 & 0.4 & 0.4 \\ 0 & 0 & 0 & 0.2 & 0.4 & 0.4 \\ 0 & 0 & 0 & 0 & 0 & 0.8 \\ 0 & 0 & 0.1 & 0.1 & 0.12 & 0.2 \end{bmatrix} \qquad (6)$$

$$\overline{R} = \begin{bmatrix} 1.0 & 0 & 0.672 & 1.008 & 0.878 & 1.718 \\ 0 & 1.0 & 0.155 & 0.357 & 1.290 & 1.546 \\ 0 & 0 & 1.172 & 0.508 & 0.878 & 1.718 \\ 0 & 0 & 0.172 & 1.508 & 0.878 & 1.718 \\ 0 & 0 & 0.153 & 0.229 & 1.336 & 1.527 \\ 0 & 0 & 0.191 & 0.286 & 0.420 & 1.908 \end{bmatrix} \qquad (7)$$

$$\overline{F} = \begin{bmatrix} 0 & 0 & 0.573 & 0.668 & 0.657 & 0.900 \\ 0 & 0 & 0.132 & 0.237 & 0.966 & 0.810 \\ 0 & 0 & 0.147 & 0.337 & 0.657 & 0.900 \\ 0 & 0 & 0.147 & 0.337 & 0.657 & 0.900 \\ 0 & 0 & 0.130 & 0.152 & 0.251 & 0.800 \\ 0 & 0 & 0.163 & 0.190 & 0.314 & 0.476 \end{bmatrix}$$

Hence, $E_{1_1}[N_2] = 0.672$, $E_{1_1}[N_3] = 1.008$, $E_{1_1}[N_4] = 0.878$, $E_{1_1}[N_5] = 1.718$ and $\mathrm{var}_{1_1}[N_2] = 0.451$, $\mathrm{var}_{1_1}[N_3] = 1.015$, $\mathrm{var}_{1_1}[N_4] = 0.697$, $\mathrm{var}_{1_1}[N_5] = 1.888$, while $E_{1_2}[N_2] = 0.155$, $E_{1_2}[N_3] = 0.357$, $E_{1_2}[N_4] = 1.290$, $E_{1_3}[N_5] = 1.546$ and $\mathrm{var}_{1_2}[N_2] = 0.184$, $\mathrm{var}_{1_2}[N_3] = 0.592$, $\mathrm{var}_{1_2}[N_4] = 0.492$, $\mathrm{var}_{1_2}[N_5] = 1.964$.

The other process characteristics discussed in Part I can be computed in much the same way as before with only minor modifications. For the total number of flow regions, N, visited by a fluid element, we use Eqs. 22 and 23 of Part I with $F_m = [F_m(1_1), \ldots, F_m(1_l), F_m(2), \ldots, F_m(r)]$. For the fraction of material, $f_A(i)$, leaving region i that never visits a specified set of regions A (see Eq. 25 of Part I), we use Eq. 26 of Part I with $f_A(r + k) = 1$ for $k = 1,\ldots,s$ instead of Eq. 27 of Part I. The computation of $F_m(i)$ is the same in Part I.

CHARACTERISTICS RELATED TO OUTLETS

Next we discuss system characteristics related to the history of particles leaving the system. Consider first the fraction of type i particles, $F(1_i,0_k)$, which exist through outlet 0_k. We know (see Eqs. 10 and 11 of Part I) how to compute the numbers $F(i,j)$ for $i = 1_1,\ldots,1_l$ and $j = 2,\ldots,r$, and now we wish to compute them for $j = 0_1,\ldots,0_r$. These are the probabilities of eventually reaching each of the absorbing states (outlets) and are called absorption probabilities. The procedure for computing them is outlined in Part I and proceeds as follows. Let $\boldsymbol{B}$ be the $((l + r - 1) \times s)$ matrix obtained from $\overline{P}$ by deleting all rows that correspond to the outlets and all columns that correspond to inlets or to flow regions. Also, let $G(i,k) = F(i,0_k)$ and $\overline{G}$ be given by

$$\overline{G} = \begin{bmatrix} F(1_1,0_1) & \cdots & F(1_1,0_1) \\ \vdots & & \vdots \\ F(1_l,0_1) & \cdots & F(1_l,0_s) \\ F(2,0_1) & \cdots & F(2,0_1) \\ \vdots & & \vdots \\ F(r,0_1) & \cdots & F(r,0_s) \end{bmatrix}$$

Then (see Çinlar, 1975, and Eq. 12 of Part I)

$$\overline{G} = \overline{R} \cdot \overline{B} \qquad (8)$$

and the first l rows of G are the fractions we are interested in.

Note that $F(1_i,0_k)$ is the fraction of type i particles that exist through outlet 0_k, not the fraction of type i particles in the outlet 0_k. To compute the latter, let X_∞ denote the terminal state of a particle, i.e., the outlet through which it exits. (If a particle exits through outlet 0_k, we shall write $X_\infty = k$.) Also, let $c_k(i)$ be the fraction of type i particles in the material leaving the system through outlet 0_k. Then $c_k(i)$ is the conditional probability that a particle entered the system through inlet i given that it leaves it through outlet k. Thus, using Bayes formula we have

$$c_k(i) = P\{X_o = 1_i | X_\infty = k\} = \frac{P\{X_o = 1_i\} P\{X_\infty = k | X_o = 1_i\}}{P\{X_\infty = k\}} \qquad (9)$$

The first term in the numerator is the initial probability $\pi(i)$ and the second term is $F(1_i,0_k)$. The denominator is the fraction of material leaving the system through outlet 0_k, which we denote by c_k. Hence Eq. 9 may be written as

$$c_k(i) = \frac{\pi(i) G(i,k)}{c_k} \qquad (10)$$

where

$$c_k = \sum_{i=1}^{l} \pi(i) G(i,k) \qquad (11)$$

Since

$$\sum_{i=1}^{l} G(i,k) = 1 \quad \text{and} \quad \pi(i) = w_o(i) / \sum_{i=1}^{\pi} w_o(i),$$

the particle flow rate through exit k is (as expected) the net flow rate through the system times c_k. The composition of each outlet stream is given by Eq. 10.

For the example of Figure 1, the computation of the two c_k's and four $c_k(i)$'s proceeds as follows. The matrix $\overline{B}$ is

$$\overline{B} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0.2 \\ 0.48 & 0 \end{bmatrix}$$

and the matrix R is given in Eq. 7 above. So, using Eq. 8 we obtain

$$\overline{G} = \begin{bmatrix} 0.824 & 0.176 \\ 0.742 & 0.258 \\ 0.824 & 0.176 \\ 0.824 & 0.176 \\ 0.733 & 0.267 \\ 0.916 & 0.084 \end{bmatrix}$$

Hence, using Eqs. 10 and 11, we obtain $c_1 = 0.783$, $c_2 = 0.217$, and $c_1(1) = 0.526$, $c_2(1) = 0.406$, $c_1(2) = 0.474$, $c_2(2) = 0.594$.

Note that traditionally, the values of c_k and $c_k(i)$ were obtained by material balance calculations over the individual flow regions for both the overall flow and individual components. But here we obtain these quantities from probability considerations by simple matrix operations. Also note that other system characteristics relating a particle's history and the outlet through which it exits can be derived using the same techniques. We shall not pursue this further except for the following, which may be of general interest in multiparticle systems.

Suppose we are interested in the number of visits to a certain region, say region j, by particles that leave the system through outlet k. Thus, we wish to compute $P\{N_j = n | X_\infty = k\}$, the conditional probability that a particle visits region j n times given that it exits the system through outlet 0_k. This, of course, is the same as the fraction of fluid in outlet 0_k, which completed exactly n passages through region j, i.e.

$$P\{N_j = n | X_\infty = k\} = \frac{\sum_{i=1}^{l} P\{X_o = 1_i\} P\{N_j = n, X_\infty = k | X_o = 1_i\}}{P\{X_\infty = k\}} = \frac{\sum_{i=1}^{l} \pi(i) P\{N_j = n, X_\infty = k | X_o = 1_i\}}{c_k}$$

Since the $\pi(i)$'s are known and c_k can be computed using Eq. 11, all we need is the second term in the numerator. For $n = 0$ this term is the probability that a particle that is initially in inlet 1_i never visits any of the regions in a set A consisting of region j and all outlets except outlet 0_k. Thus

$$P\{N_j = 0, X_\infty = k | X_o = 1_i\} = f_A(1_i)$$

In general, we have

$$P\{N_j{=}n, X_\infty{=}k | X_o = 1_i\} = \begin{cases} f_A(1_i) & (n = 0) \\ F(1_i,j)F^{n-1}(j,j)F_j(j,k) & (n = 1,2,\ldots) \end{cases}$$

where

$$F_j(j,k) = \sum_{\gamma \notin A} p(j,\gamma) f_A(\gamma) \tag{12}$$

Since we know how to compute $f_A(\gamma)$, we can now write the desired result in terms of known quantities:

$$P\{N_j = n | X_\infty = k\} = \begin{cases} \dfrac{1}{c_k} \sum_{i=1}^{l} \pi(i) f_A(1_i) & (n = 0) \\ \dfrac{1}{c_k} \sum_{i=1}^{l} \pi(i) F(1_i,j) F(j,j)^{n-1} F_j(j,k) & (n \geq 1) \end{cases} \tag{13}$$

with $F_j(j,k)$ given in Eq. 12.

To illustrate this computation for the system of Figure 1, let us compute the fraction of material leaving the system through exit 0_1, which visited region 3 n times, $P(N_3 = n, X_\infty = 0_1)$. Here, $\pi(1_1) = \pi(1_2) = 0.5$, and the following values were calculated earlier: $c_1 = 0.783$, $F(1_1,3) = 0.668$, $F(1_2,3) = 0.237$, and $F(3,3) = 0.337$. The set A consists of flow region 3 and exit 0_1, and the values of $f_A(\gamma)$ to be used in Eqs. 12 and 13 can be found by solving the following equations (see Part I):

$$f_A(1_1) = 0.5 f_A(2)$$
$$f_A(1_2) = 0.9 f_A(4)$$
$$f_A(2) = 0.4 f_A(4) + 0.4 f_A(5)$$
$$f_A(4) = 0.8 f_A(5) + 0.2 f_A(0_2)$$
$$f_A(5) = 0.1 f_A(2) + 0.12 f_A(4) + 0.2 f_A(5)$$
$$f_A(0_2) = 1$$

The solution is $f_A(1_1) = 0.064$, $f_A(1_2) = 0.228$, $f_A(2) = 0.128$, $f_A(4) = 0.253$, $f_A(5) = 0.0665$. From these, using Eq. 12 we have $F_3(3,0_1) = 0.4 f_A(4) + 0.4 f_A(5) = 0.128$, and from Eq. 13 we have

$$P(N_3{=}n | X_\infty{=}1) = \begin{cases} 0.146 & n = 0 \\ (0.578)(0.128)(0.337)^{n-1} & n = 1,2,\ldots \end{cases}$$

REGIONAL RESIDENCE TIMES

We now turn to particle residence time in region j. Let $H_{i,j}(x)$ be the distribution function of the duration of a single visit to region j by a type i particle, and let $\mu_j(i)$ and $\sigma_j^2(i)$ be the mean and variance, respectively, of this duration.

The derivation of an expression for the total regional residence time, in region j for type i particles, is similar to that given in Part II except that here one has to replace p_j with $p_j(i)$ (see Eq. 3) and $H_j(x)$ by $H_{i,j}(x)$. Thus, the joint distribution of N_j and T_j for type i particles

$$G_{i,j}(n,t) = P\{N_j{=}n, T_j \leq t | X_o = 1_i\}$$

is given by

$$G_{i,j}(n,t) = \begin{cases} 1 - p_j(i) & (n = 0) \\ p_j(i)(1 - q_j) q_j^{n-1} H_{i,j}^{*n}(t) & (n = 1,2,\ldots) \end{cases} \tag{14}$$

(see Part II). The total residence time distribution of type i particle in region j

$$G_{i,j}(t) = P\{T_j \leq t | X_o = 1_i\}$$

is given by

$$G_{i,j}(t) = (1 - p_j(i)) + \sum_{n=1}^{\infty} p_j(i)(1 - q_j) q_j^{n-1} H_{i,j}^{*n}(t), \qquad (t \geq 0) \tag{15}$$

(see Eq. 14 of Part II), and the mean total regional time of type i particles in region j is

$$E[T_j | X_o = 1_i] = \frac{p_j(i)\mu_j(i)}{1 - q_j} = E[N_j | X_o = 1_i]\mu_j(i) \tag{16}$$

Also, the covariance of the number of visits to region j and the total regional residence time in this region by a type i particle is

$$\mathrm{Cov}[N_j, T_j | X_o = 1_i] = \frac{\mu_j(i)[p_j(i) + p_j(i)q_j - p_j^2(i)]}{(1 - q_j)^2}$$

The correlation coefficient of N_j and T_j for type i particles is

$$\rho_i(N_j, T_j) = 1 + \left[\frac{p_j(i)(1 - q_j)\sigma_j^2(i)}{(1 + q_j - p_j(i)\mu_j^2(i)}\right]^{-1/2}$$

From Eq. 15 we also find the density of $G_{i,j}(t)$:

$$g_{i,j}(t) = (1 - p_j(i))\delta(o) + \sum_{n=1}^{\infty} p_j(i)(1 - q_j) q_j^{n-1} h_{i,j}^{*n}(t) \tag{17}$$

where $h_{i,j}(t)$ is the density of the residence time in region j of type i particles.

LOCAL FLOW RATES AND MATERIAL COMPOSITIONS

Let $w_o(i)$ be the flow rate through inlet 1_i, i.e., input of type i particles. Let w_o be the net flow rate through the system so that

$$w_o = \sum_{i=1} w_o(i)$$

Note that $w_o(i)$ denotes the number of type i particles entering the system in unit time. Thus, w_o is the total number of particles entering (or leaving) the system in unit time. These are similar to molar flow rates encountered in many instances. Let $w_j(i)$ be the flow rate of type i particles through region j and

$$w_j = \sum_{i=1}^{l} w_j(i)$$

be the total net flow rate through that region. Then using the same methods as in Part II, we obtain that for each particle type

$$w_j(i) = E[N_j | X_o{=}1_i] w_o(i) \tag{18}$$

and

$$w_j = w_o E[N_j] \tag{19}$$

where

$$E[N_j] = \sum_{i}^{l} \pi(i)R(1_i,j) \tag{20}$$

The last relation can be derived by the method of combining all inlets and outlets, as described in the introduction, and then applying Eq. 19 of Part II to the new system. Alternatively, one can formally sum Eq. 18 over all i and write

$$w_j = \sum_{i=1}^{l} w_j(i) = \sum_{i=1}^{l} \frac{E[N_j|X_o=1_i]w_o(i)}{w_o} w_o$$
$$= w_o \sum_{i=1}^{l} E[N_j|X_o=1_i]\pi(i) = w_o E[N_j]$$

As we see, for multiparticle systems, local flow rates are equal to the net flow rate through the system times the expected number of visits to the local zone of interest. *This basic result applies to each particle type as well as to the aggregate of all particles in the system.* Also, the decomposition method discussed in Part II can be used here as well to prove that Eqs. 18 and 19 are true for any general system *irrespective of the number of inlets and outlets to each flow region.*

These last results lead to some important relations on local material composition. Let $y_j(i)$ be the fraction of type i particles in the inlet to region j. Thus, for each i and j we must have

$$y_j(i) = \frac{w_j(i)}{w_j} \tag{21}$$

Now using Eqs. 18 and 19 in the last relation we obtain

$$y_j(i) = \frac{w_o(i)E[N_j|X_o = 1_i]}{w_o E[N_j]}$$

which is the same as

$$y_j(i) = \frac{\pi(i)E[N_j|X_o=1_i]}{E[N_j]} \tag{22}$$

Thus, the fraction of type i material in the inlet (or outlet) of region j is equal to the fraction of type i material in the total input times the ratio of the expected number of visits to region j by type i particles to the overall expected number of visits to that region. The last relation can also be written in a different form as follows. From Eq. 20

$$E[N_j] = \sum_{i=1}^{l} \pi(i)E[N_j|X_o=1_i]$$

and (by analogy to Eq. 18 of Part I)

$$E[N_j|X_o=1_i] = \frac{p_j(i)}{1 - q_i}$$

Hence

$$y_j(i) = \frac{\pi(i)p_j(i)}{p_j} \tag{23}$$

where

$$p_j = \sum_{i=1}^{l} \pi(i)p_j(i)$$

In other words, the fraction of type i material in region j is the same as the fraction of this material in the total input times the ratio between the probability that a type i particle will ever reach region j to the overall probability that any entering particle will ever visit region j.

Now, consider the material composition inside flow region j. When all particle types obey the same laws of movements in the region, the internal composition inside the region is the same as its inlet (or outlet) composition. This is because the mean residence time inside the region is the same for all particle types. However, in applications there are many systems where sojourn times in a region vary among particle types (for example, due to absorption) while movements between zones are the same for all particles. Below we derive expressions for material composition inside flow regions for this more general case.

To start with, note that for the present situation, Eqs. 18 to 23 all hold true, since their proof is not affected by differences in sojourn times. Let $z_j(i)$ denote the fraction of type i particles inside region j. Also, let $V_j(i)$ be the number of type i particles in region j, and V_j the total number of particles in region j. Then

$$z_j(i) = \frac{V_j(i)}{V_j}$$

Also, for each particle type

$$\mu_j(i) = \frac{V_j(i)}{w_j(i)}$$

The overall mean duration of a visit in region j is given by

$$\mu_j = \frac{V_j}{w_j}$$

and can be written as the sum over all i of the fraction of type i particles entering region j time $\mu_j(i)$:

$$\mu_j = \sum_{i=1}^{l} \frac{w_j(i)}{w_j} \mu_j(i) = \sum_{i=1}^{l} y_j(i)\mu_j(i) \tag{24}$$

From this we immediately obtain

$$z_j(i) = \frac{y_j(i)\mu_j(i)}{\mu_j} \tag{25}$$

Note that if $\mu_j(i) = \mu_j$ for all i, $z_j(i) = y_j(i)$ and that $\Sigma_i z_j(i) = 1$, as it should. Finally, using Eqs. 22 and 23 we can rewrite Eq. 25 as

$$z_j(i) = \frac{\pi(i)E[N_j|X_o=i]\mu_j(i)}{E[N_j]\mu_j} \tag{26}$$

or

$$z_j(i) = \frac{\pi(i)p_j(i)\mu_j(i)}{p_j\mu_j} \tag{27}$$

Equation 25 is a fundamental relationship that ties together the overall composition inside a region and the composition at the region's outlet (or inlet). It indicates that whenever the mean duration of a visit to the region is different among the different fluid types, the internal and exit compositions are different. This property can be exploited experimentally in several ways: First, when internal and exit compositions of a given region ($z_j(i)$ and $y_j(i)$) can be measured for all components i, the mean sojourn times in the region for each particle type can be calculated by solving the following system of linear equations:

$$z_j(i) = \frac{y_j(i)\mu_j(i)}{\Sigma y_j(i)\mu_j(i)} \qquad i = 1,2,\ldots,l$$

Thus, for multifluid systems, the individual mean regional sojourn times can be determined without employing a tracer technique. Second, Eqs. 25, 26, and 27 can also be used to determine (or verify) model parameters, such as p_j, $p_j(i)$, or $E[N_j]$, without measuring $N_j(i)$ directly.

Finally, it is worth noting that in this paper we considered a system (or a model) whose structure is known and proceeded to calculate different process characteristics. In practice, the internal structure of a system may not be known. For such cases, by measuring the number of visits to flow regions as well as the internal and exit compositions, and by using Eqs. 4, 10, 16, and 25, different system parameters can be calculated or reliable models can be constructed. These points will be discussed elsewhere.

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NOTATION

$\overline{B}$ = matrix of transition probabilities from a transient state to an absorbing state

c_k = fraction of material leaving the system through outlet k
$c_k(i)$ = fraction of type i particles leaving the system through outlet k
$F(i,j)$ = probability of a particle leaving region i will ever reach region j (see Eq. 10 of Part I)
$F_j(j,k)$ = probability of a particle leaving region j will ever reach outlet k without returning to region j
$\overline{F}$ = matrix whose entries are $F(i,j)$
$f_A(i)$ = probability of a particle leaving region i will never visit any of the flow regions in set A
$G(i,k)$ = probability of a particle moving in one step from a transient state i to an absorbing state k
$\overline{G}$ = matrix whose entries are $G(i,k)$
$G_{i,j}(n,t)$ = probability that a type i particle visits in region j n times and resides in it no more than t time units
$G_{i,j}(t)$ = distribution of total residence time of type i particle in region j
$H_{i,j}(t)$ = distribution function of a duration of a single visit to region j by a type i particle
$h_{i,j}(t)$ = density function of $H_{i,j}(x)$
l = number of inlets
N_j = number of visits to region j by a particle
O_k = outlet k
I_i = inlet i
P = matrix of transition probabilities
$p(i,j)$ = probability that a particle entering region j immediately after leaving region i
$p_j(i)$ = probability that a particle leaving region i will ever visit region j
q_j = probability of a particle leaving region j will ever return to region j
$\overline{Q}$ = matrix obtained from P by deleting all rows and columns corresponding to the outlets
Q_A = matrix obtained from P by deleting all rows and columns corresponding to the regions in a specified set A
$R(i,j)$ = expected number of visits to region j by a particle that is initially in region i
$\overline{R}$ = matrix whose entries are $R(i,j)$
$r-1$ = number of flow regions
s = number of outlets
T_j = total residence time of a particle in region j
t = time
V_j = volume of region j
V_o = total volume of the system
$V_j(i)$ = volume of type i particles in region j
w_j = total particle flow rate through region j
$w_j(i)$ = particle flow rate of type i fluid through region j
w_o = total particle flow rate through the system
$w_o(i)$ = particle flow rate through inlet i
X_n = random variable indicating the state (region) of a particle in its nth step
X_∞ = final state of a particle
$y_j(i)$ = fraction of type i particles in the inlet (and outlet) to region j
$z_j(i)$ = fraction of type i particles inside region j

GREEK LETTERS

μ_j = mean duration of a visit to region j
$\mu_j(i)$ = mean duration of a visit to region j by a type i particle
$\pi(i)$ = fraction of type i particles in the inlet to the system
$\overline{\pi}$ = vectors whose entries are (i)
$\sigma_j^2(i)$ = variance of the duration of a visit of type i particle in region j

LITERATURE CITED

Çinlar, E., *Introduction to Stochastic Processes*, Prentice-Hall, Englewood Cliffs, NJ (1975).

Mann, U., and M. Rubinovitch, "On Measuring Local Flow Rates in Process Units," *Ind. Eng. Chem. Process Des. Develop.*, **22**, 545 (1983).

Rubinovitch, M., and U. Mann, "A Single Particle Approach for Analyzing Flow Systems: I. Visits to Flow Regions," *AIChE J.*, **29**(4), 658 (1983a).

———, "A Single Particle Approach for Analyzing Flow Systems: II. Regional Residence Times and Local Flow Rates," *AIChE J.*, **29**(4), 663 (1983b).

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