# Single-Particle Approach for Analyzing Flow Systems

## Part I: Visits to Flow Regions

A methodology is presented for characterizing and analyzing general continuous flow system with special emphasis on particulate processes. The methodology is based on describing the history of individual particles (or fluid elements) in the process. The movements of particles are expressed in terms of the flow regions they visit using a Markov chain presentation. Explicit expressions as well as computational methods are derived for various process characteristics of interest. These include the distributions, means and variances of: the number of visits to any specified flow region; the total number of regions visited; and the number of visits to any specified set of regions. This methodology yields information on bulk properties as well as on individual particle behavior and deviations among particles.

**MICHAEL RUBINOVITCH**

Industrial Engineering and Management
Technion—Israel Institute of Technology
Haifa, Israel

**UZI MANN**

Department of Chemical Engineering
Texas Tech University
Lubbock, TX 79409

### SCOPE

Traditionally, chemical processes are analyzed by using the continuum approach, and classical mathematical tools can be employed to describe physical and chemical changes using conservation equations and rate expressions. The continuum assumption is made despite the realization that all fluids consist of discrete elements. It is justified for gases and liquids, since any volume element contains a huge number of molecules which may be lumped together to obtain the bulk properties. For particulate processes, however, the particulate phase consists of relatively large elements, which are usually not identical. A volume unit contains a finite (and in many cases small) number of particles; consequently, the continuum assumption is not physically justified and may lead to oversimplified and unrealistic process description. Furthermore, even when justified, the continuum approach does not provide information on the deviations among particles.

In this series of papers we use a different approach to develop a methodology for analyzing flow systems. The approach is based on describing the movements of individual particles in a system as a stochastic process governed by the probabilistic laws of these movements. Then, using the machinery of probability theory we derive explicit results for some system characteristics. The stoichastic process we use in this paper is a discrete time Markov chain. Most of the results are related to number of times a particle visits (or passes through) a specified region in the system.

### CONCLUSIONS AND SIGNIFICANCE

The trajectory of a particle in a process is characterized in terms of the flow regions it visits and the number of times it visits various flow regions. We derive relations and describe computational methods for the distributions, means and variances of the following process characteristics: (a) the number of visits to a specified flow region; (b) the number of visits to a specified flow region by a particle leaving another specified flow region; and (c) the total number of regions visited by a particle as it passes through the system. We also calculate the fraction of particles ever visiting (or avoiding) a specified set of flow regions.

These characteristics have not been considered in chemical engineering. They are important in processes and operations where particle properties are directly related to number of visits to a specified region. Furthermore, these results also lead to other important system characteristics. In a subsequent paper, we show how local flow rates and residence times in specified regions can be derived with the use of the expressions obtained here.

---

### INTRODUCTION

In this paper we develop a Markov chain model for analyzing general flow systems with special attention to particulate processes. The Markov chain model is used here to keep track of the movements of a single particle as it passes through the system in terms of the flow regions it visits.

Several investigators have used stochastic formulation in chemical engineering studies but mainly to construct flow models and calculate residence time distributions. Seinfeld and Lapidus (1974) summarize earlier works in this area. More recent works are done by Schmalzer and Hoelscher (1977), Srinivasan and Mehta (1972), and Raghuraman and Mohan (1975). However, the use of

stochastic models to describe the history of particles, or a fluid elements, for purposes other than RTD calculation has so far been rather limited. (See, however, Mann et al., 1979, and Mann and Rubinovitch, 1981.)

In this paper we describe in detail the basic model and its underlying assumptions and show how to compute some new system characteristics of interest. These concepts and results will be used in subsequent papers for further analysis. It is important to note that, although the probabilistic approach used here is based on analyzing the history of single particles, the results are applicable to processes of homogeneous fluids since gases and liquids can be viewed as a particulate phase with a huge number of identical particles (molecules).

## BASIC MODEL AND ITS ASSOCIATED MARKOV CHAIN

Consider a general flow system or model with several flow regions which are interconnected in an arbitrary way. We assume that the system is at steady state; i.e., flow rates and patterns do not change with time. We also assume that the system and each flow region have only one inlet and one outlet. There are no other restrictions on the structure of the system or internal mixing and flow patterns inside each flow region; they all may be arbitrary. (In a subsequent paper we shall show how these assumptions can be relaxed.) Figure 1 shows a flow diagram for one such system. We shall use it as an example throughout the exposition. This example was constructed to include elements which are frequently encountered in chemical engineering processes: split streams, recycles, bypasses and interconnections between recycle loops.

Let us assign the number 1 to the inlet, the numbers 2, 3, . . . , $r$ to the various flow regions, and the number $r + 1$ to the outlet. Let $V_2, \ldots, V_r$ be the volumes of the respective flow regions and $V = V_2 + \ldots + V_r$ be the total volume of the system. Now focus attention on one particle and its movement in the system. Its *initial state* is 1 and we denote this by $X_o = 1$. Then upon entering the system the particle will enter one of the flow regions. If this is region $i$, we say that *on its first step the particle is at state* $i$, and write $X_1 = i$. Similarly, if the $n$th flow region it enters is region $j$, $X_n = j$ and we say that *on its nth step* the particle is in state $j$. If at some step, say step number $\nu$, the particle leaves the system, we write $X_\nu = r + 1$ and then $X_n = r + 1$ for all $n \geq \nu$.

The sequence $\{X_n; n = 0,1, \ldots\}$ is a discrete time, discrete state space stochastic process, and its trajectories give a complete account of the particle's movement in the system in terms of the flow regions it visits. The key to our analysis is the fact that for most practical systems this is a Markov chain. This is so since the probability that a particle will, on its $(n + 1)$st step enter a specified region, given its complete history up to and including the $n$th step, depends only on its state in the $n$th step. In other words, once a particle is in a given flow region its future movements do not depend on past movements. Formally, for all $n \geq 0$ and all $j$,

$$P\{X_{n+1} = j | X_o, X_1, \ldots, X_n\} = P\{X_{n+1} = j | X_n\} \qquad (1)$$

(See, for example, Çinlar, 1975.) Furthermore, in most practical situations the righthand side of Eq. 1 is independent of $n$, i.e.

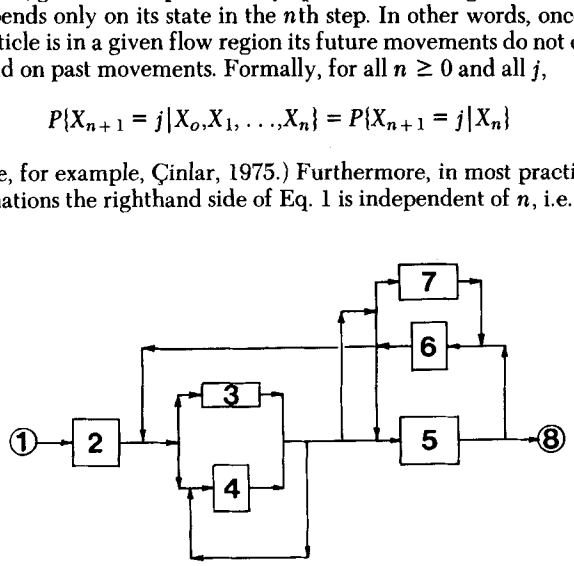


Figure 1. Schematic description of an arbitrary system.

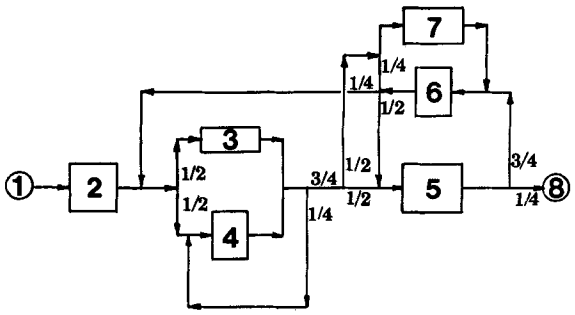


Figure 2. Example system.

$$P\{X_{n+1} = j | X_n = i\} = P\{X_1 = j | X_o = i\} \qquad (2)$$

for all $n$. A process which satisfies Eq. 1 is a *Markov chain*. When Eq. 2 is also satisfied it is a Markov chain with *stationary transition probabilities*. Henceforth we shall assume that both Eqs. 1 and 2 hold true. Then, using standard notation we write

$$P(i,j) = P\{X_{n+1} = j | X_n = i\}, \qquad (3)$$

for $i,j, = 1, \ldots, r + 1$. This is the *transition probability* from state $i$ to state $j$ and

$$\mathbf{P} = \begin{bmatrix} P(1,1) & \ldots . P(1,r+1) \\ \vdots & \\ P(r+1,1) & \ldots P(r+1,r+1) \end{bmatrix} \qquad (4)$$

is the *matrix of transition probabilities*. The $(i,j)$th entry of this matrix is the probability that a particle which exists from region $i$, will in one step, enter region $j$. $P(i,j)$ is also the fraction of material leaving region $i$ which immediately enters region $j$. Below we assume that $\mathbf{P}$ is known.

Suppose that in the example fractions of material at each split point are as indicated in Figure 2. Then the matrix $\mathbf{P}$ is:

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 3/8 & 0 & 3/8 & 0 \\ 0 & 0 & 0 & 1/4 & 3/8 & 0 & 3/8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3/4 & 0 & 1/4 \\ 0 & 0 & 1/8 & 1/8 & 1/2 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \qquad (5)$$

Once we have presented the movement of particles in the system in terms of the Markov chain $X$, the theory of Markov chains is at our disposal for deriving various system characteristics which are of practical and theoretical interest. In order to do this we shall need some basic terminology and results on Markov chains. These are now briefly reviewed. For references, see Çinlar (1975) or Keneny, Snell and Knapp (1966). As much as possible we shall follow the notation of Çinlar (1975). Other references are Feller (1971) and Chung (1967). See also Seinfeld and Lapidus (1974).

Let $\{X = X_n; n = 0,1,2, \ldots\}$ be a Markov chain with stationary transition probabilities on the state space $E = \{1,2, \ldots, r + s\}$, where $r$ and $s$ are positive integers. (We choose this state space since in subsequent papers we consider systems with several outlets. Then $s$ will be the number of outlets.) Let

$$\pi(i) = P\{X_o = i\} \qquad (i \in E),$$

and $\boldsymbol{\pi} = [\pi(1), \ldots, \pi(r + s)]$. The vector $\boldsymbol{\pi}$ is called the *initial distribution*, and its entries must satisfy $\pi(i) \geq 0$ and $\Sigma\pi(i) = 1$. (Whenever we write $\Sigma$ without limits, the summation is over all elements of $E$.) This vector determines the starting point of the Markov chain $X$.

A state $j$ is called *absorbing* whenever $P(j,j) = 1$. A particle which reaches an absorbing state stays there forever. In our case states $r + 1, \ldots, r + s$ are absorbing. A state $j$ is called *transient*

whenever the total number of visits to this state is finite with probability one. In other words, from some point onwards a particle never enters a transient state. In our case states $1, \ldots, r$, are transient.

It follows that all matrices **P** we shall deal with may always be written as:

$$\mathbf{P} = \begin{bmatrix} \mathbf{Q} & \mathbf{B} \\ \mathbf{O} & \mathbf{I} \end{bmatrix}, \tag{6}$$

where **Q** is an $(r \times r)$ matrix whose entries are transition probabilities from a transient state to a transient state. **B** is an $(r \times s)$ matrix whose entries are transition probabilities from transient to absorbing states, **O** is an $(r \times s)$ zero matrix whose entries are the transition probabilities from absorbing states to transient states, and **I** is an $(s \times s)$ identity matrix. (We shall use **I** for all identity matrices and in each case dimensions should be determined so that the expressions make sense.) [In Markov chain literature it is customary to label states so that recurrent (absorbing) states correspond to the top rows of $P$. In this paper states are labeled differently and some care should be exercised when looking up the references. For example, the representation of Eq. 6 is a different format than that given in Çinlar (1975)].

A typical evolution of our Markov chain consists of transitions from one transient state (flow region) to another until, eventually, an absorbing state (outlet) is reached. Let $N$ be the number of states visited before absorption (including the visit to the origin) and let $N_j$ be the number of visits to region $j$ before absorption occurs. Then $N = N_1 + N_2 + \ldots + N_r$.

The distribution of these random variables will, in general, depend on the initial state of the chain and hence we shall be interested in the conditional probabilities, $P\{N_j = m | X_o = i\}$; i.e., the probability that $N_j = m$ given that the initial state is $i$. We shall write $P_i\{N_j = m\}$ for this probability. Similarly $E_i[N_j] = E[N_j | X_o = i]$ and $\mathrm{Var}_i[N_j] = \mathrm{Var}[N_j | X_o = i]$ will denote, respectively, the mean and variance of $N_j$ given that the initial state is $i$.

For $i,j = 1, \ldots, r$ let

$$R(i,j) = E_i[N_j], \tag{7}$$

and **R** be the matrix with entries $R(i,j)$. Then it is known that

$$\mathbf{R} = (\mathbf{I} - \mathbf{Q})^{-1}, \tag{8}$$

where **Q** is the matrix appearing in Eq. 6. Also, for $i,j \in E$ let

$$F(i,j) = P_i\{X_m = j \quad \text{for some } m = 1,2, \ldots\}, \tag{9}$$

be the probability of ever reaching state $j$ if the initial state is $i$. In particular $F(j,j)$ is the probability of ever returning to $j$ when the initial state is $j$. For $i,j = 1, \ldots, r$ $F(i,j)$ can be computed using the relations

$$F(j,j) = 1 - \frac{1}{R(j,j)} \tag{10}$$

$$F(i,j) = \frac{R(i,j)}{R(j,j)} \qquad (i \neq j). \tag{11}$$

To compute $F(i,j)$ for $i = 1, \ldots, r$ and $j = r+1, \ldots, r+s$, let

$$\mathbf{G} = \begin{bmatrix} F(1,r+1) \ldots F(1,r+s) \\ \vdots \\ F(r,r+1) \ldots F(r,r+s) \end{bmatrix}$$

then

$$\mathbf{G} = \mathbf{R} \cdot \mathbf{B}, \tag{12}$$

where **R** is given by Eq. 8 and **B** is the matrix appearing in Eq. 6. Clearly, $F(i,j) = 0$ for $i = r+1, \ldots, r+s$ and $j = 1,2, \ldots, r+s$ and $j \neq i$.

Now we can write down the distribution of $N_j$. For $j = 1, \ldots, r$ this is

$$P_j\{N_j = m\} = F(j,j)^{m-1}(1 - F(j,j)) \quad m = 1,2, \ldots, \tag{13}$$

and for $i = 1, \ldots, r$ and $i \neq j$ it is

$$P_i\{N_j = m\} = \begin{cases} 1 - F(i,j) & m = 0 \\ F(i,j)F(j,j)^{m-1}(1 - F(j,j)) & m = 1,2, \ldots \end{cases} \tag{14}$$

These are the basics we shall need. Further results on Markov chains will be called upon when needed.

## NUMBER OF VISITS TO A SPECIFIED FLOW REGION

Consider the general flow system with one inlet (Region 1) and one outlet ($s = 1$) and its associated Markov chain. The first characteristic we consider is the fraction of particles which pass exactly $m$ times through region $j$. This is $P_1(N_j = m)$ which is obtained directly from Eq. 14, *viz.*

$$P_1\{N_j = m\} = \begin{cases} 1 - p_j & m = 0 \\ p_j q_j^{m-1}(1 - q_j) & m = 1,2, \ldots \end{cases} \tag{15}$$

where $p_j$ is the fraction of particles which pass at least once through region $j$, and $q_j$ is the fraction of particles leaving region $j$ which eventually return to $j$. In other words

$$p_j = F(1,j) \qquad q_j = F(j,j). \tag{16}$$

The mean number of visits to region $j$ is

$$\mu_N(j) = E_1[N_j] = R(1,j). \tag{17}$$

We shall later need expressions for the mean and variance of $N_j$ in terms of $p_j$ and $q_j$. These can be evaluated directly from Eq. 15, i.e.,

$$\mu_N(j) = E_1[N_j] = \sum_{m=0}^{\infty} m P_1\{N_j = m\} = \frac{p_j}{1 - q_j} \tag{18}$$

$$\sigma_N^2(j) = \frac{p_j(1 + q_j - p_j)}{(1 - q_j)^2} \tag{19}$$

A complete analysis for the number of visits to flow regions will proceed as follows. Start with the matrix **P** and obtain matrix **Q** of Eq. 6 by deleting its last row and column. Then compute $\mathbf{R} = (\mathbf{I} - \mathbf{Q})^{-1}$ (Eq. 8) and $F(j,j)$ and $F(i,j)$ using Eqs. 10 and 11. Next obtain $p_j$ and $q_j$ using Eq. 16 and then compute the desired system characteristics according to Eqs. 15, 17, 18 and 19. For the example of Figure 2,

$$\mathbf{R} = \begin{bmatrix} 1 & 1 & 1.2 & 2 & 4 & 5.6 & 2.6 \\ 0 & 1 & 1.2 & 2 & 4 & 5.6 & 2.6 \\ 0 & 0 & 1.7 & 1.5 & 4 & 5.6 & 2.6 \\ 0 & 0 & 0.7 & 2.5 & 4 & 5.6 & 2.6 \\ 0 & 0 & 0.6 & 1 & 4 & 4.8 & 1.8 \\ 0 & 0 & 0.8 & 1.333 & 4 & 6.4 & 2.4 \\ 0 & 0 & 0.8 & 1.333 & 4 & 6.4 & 3.4, \end{bmatrix}$$

$p_2 = 1$ $\quad p_3 = 0.706$ $\quad p_4 = 0.8$
$p_5 = 1$ $\quad p_6 = 0.875$ $\quad p_7 = 0.765$
$q_2 = 0$ $\quad q_3 = 0.412$ $\quad q_4 = 0.6$
$q_5 = 0.75$ $\quad q_6 = 0.844$ $\quad q_7 = 0.706$

Hence,

$\mu_N(1) = 1$ $\quad \sigma_N^2(1) = 0$
$\mu_N(2) = 1$ $\quad \sigma_N^2(2) = 0$
$\mu_N(3) = 1.2$ $\quad \sigma_N^2(3) = 1.440$
$\mu_N(4) = 2$ $\quad \sigma_N^2(4) = 4$
$\mu_N(5) = 4$ $\quad \sigma_N^2(5) = 12$
$\mu_N(6) = 5.6$ $\quad \sigma_N^2(6) = 34.7$
$\mu_N(7) = 2.6$ $\quad \sigma_N^2(7) = 8.32$

As we see, interesting characteristics of rather complicated systems can be computed with the simple machinery we have at hand. But the results that this can provide are not limited just to these computations. Suppose for example that we are interested in studying the effect of the recycle to Region 4. We do this by comparing the mean number of visits to Region 4 and Region 3.

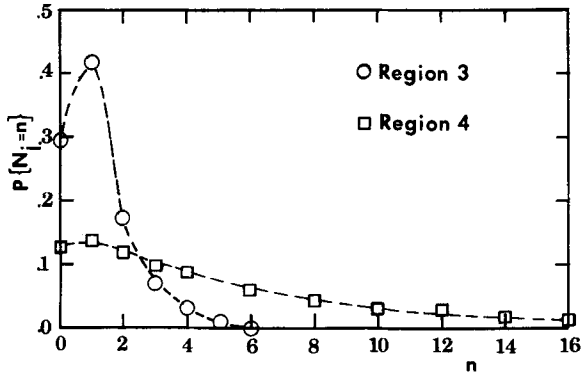


Figure 3. Distributions of number of visits to Regions 3 and 4.

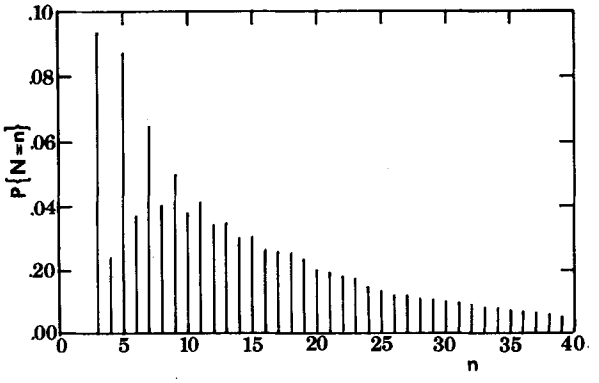


Figure 4. Distribution of total number of flow regions visited.

As we see, 70.6% of all particles pass, at least once through Region 3 while 80% pass, at least once, through Region 4. The mean number of passages through Region 3 is 1.2 while it is 4 for Region 4. On the other hand, the variability in the number of passages through these regions, as measured by the coefficient of variation, is the same since $\sigma_N(3)/\mu_N(3) = 1$ and $\sigma_N(4)/\mu_N(4) = 1$. The complete picture on the number of visits to these two regions is of course, given by the distributions of $N_3$ and $N_4$. These are

$$p_1\{N_3 = m\} = \begin{cases} 0.294 & m = 0 \\ 0.415 \times 0.412^{m-1} & m = 1,2,\ldots \end{cases}$$

$$P_1\{N_4 = m\} = \begin{cases} 0.125 & m = 0 \\ 0.137 \times 0.844^{m-1} & m = 1,2,\ldots \end{cases}$$

and their frequency distributions are shown in Fig. 3.

We conclude the discussion on number of visits to a given region with two comments. First, note that the matrix **R** is not just a tool for computing $p_j$ and $q_i$. In many situations all its entries may be of interest since $R(i,j)$ is the mean number of passages through region $j$ by a particle which exits from region $i$. Similarly, all the entries of matrix **F** may be of independent interest since $F(i,j)$ is the fraction of material leaving region $i$ which passes at least once through region $j$. The second comment concerns the computations of $\sigma_N^2(j)$. Once $p_j$ and $q_j$ are known these can be computed using Eq. 19. However, there is a shorter way to do this. Let

$$\boldsymbol{\sigma}_n^2 = \begin{bmatrix} \mathrm{Var}_1[N_1] \ldots \mathrm{Var}_1[N_r] \\ \vdots \\ \mathrm{Var}_r[N_1] \ldots \mathrm{Var}_r[N_r] \end{bmatrix},$$

then (Kemeny, Snell and Knapp, 1966)

$$\boldsymbol{\sigma}_n^2 = \mathbf{R}(2\mathbf{R}_{dg} - \mathbf{I}) - \mathbf{R}_{sq} \tag{20}$$

where $\mathbf{R}_{dg}$ is the matrix obtained from **R** by replacing all non-diagonal elements with zeros, and $\mathbf{R}_{sq}$ is the matrix obtained by squaring each entry in **R**.

## TOTAL NUMBER OF REGIONS VISITED

In the previous section we considered the number of visits to a specified flow region. There are however systems where the same change takes place in all flow regions. Then one may be interested in the total number of visits to all flow regions. This is represented by the random variable $N = N_1 + \ldots + N_r$. We shall now show how to compute the distribution and moments of N. The computation of the mean of $N$ is easy since

$$E_1[N] = \sum_{j=1}^{r} E_1(j) = \sum_{j=1}^{r} R(1,j).$$

More generally, if $E_i[N]$ is the mean number of passages through all flow regions by a particle which exits from region $i$ then

$$E_i[N] = \sum_{j=1}^{r} R(i,j). \tag{21}$$

For the distribution function of $N$, let $F_m(i) = P_i\{N = m\}$ be the fraction of material leaving region $i$ which, after leaving that region, completes $m$ passages through flow regions before leaving the system. Then $F_1(i)$ is the probability that a particle leaving region $i$ moves directly to the outlet; i.e., $F_1(i) = P(i,r+1)$. For $m \geq 2$ $F_m(i)$ is given by the probability that the particle moves to some region other than the outlet and then visits $m-1$ regions before leaving the system. This leads to the following recursive equations:

$$F_m(i) = \begin{cases} P(i,r+1) & m = 1 \\ \sum_{j=1}^{r} P(i,j)F_{m-1}(j) & m = 2,3,\ldots \end{cases} \tag{22}$$

In matrix notation let $\mathbf{F}_m = [F_m(1),\ldots,F_m(r)]^t$, then $\mathbf{F}_1$ is the last column of **P** with its last entry deleted and,

$$\mathbf{F}_m = \mathbf{Q}\mathbf{F}_{m-1} = \mathbf{Q}^{m-1}\mathbf{F}_1 = \mathbf{Q}^{m-1}\begin{bmatrix} P(1,r+1) \\ \vdots \\ P(r,r+1) \end{bmatrix}. \tag{23}$$

In practice one would either solve this analytically or evaluate $\mathbf{F}_m$ numerically for as many $m$ values as needed. In any case, the expressions for the means $E_i[N]$ are known (Eq. 21) and the variances could be computed using

$$\begin{bmatrix} \mathrm{Var}_1[N] \\ \vdots \\ \mathrm{Var}_r[N] \end{bmatrix} = (2\mathbf{R} - \mathbf{I})\cdot\mathbf{R}\cdot\mathbf{1} - (\mathbf{R}\cdot\mathbf{1})_{sq}, \tag{24}$$

where $(\mathbf{R}\cdot\mathbf{1})_{sq}$ is the $(r \times 1)$ vector whose $i$th entry is

$$\sum_{j=1}^{r} R(i,j)^2$$

To illustrate the use of Eqs. 22 and 23 we calculate here the distribution of the total number of regions visited by a particle passing through the system shown in Fig. 2. For this case $i = 1$ (the inlet) and $\mathbf{F}_1$ is a seven element vector, obtained from the last column of Eq. 5, whose fifth element is .25 and all the others are zero. We can now calculate successively vectors $\mathbf{F}_2$, $\mathbf{F}_3$, ... by multiplying matrix **Q** (obtained from Eq. 5 by deleting the last row and last column) with each vector i.e., $\mathbf{F}_m = \mathbf{Q}\cdot\mathbf{F}_{m-1}$. The first elements in these vectors are $\mathbf{F}_m$ (1), each gives the probability that particle passes through $m$ flow regions during its passage through the system. Figure 4 shows this distribution.

## NUMBER OF VISITS TO A SET OF FLOW REGIONS

The methods presented so far can be refined to produce results on the probability of ever visiting (or avoiding) a specified set of

flow regions. Suppose, for example, that the system has regions where a reaction takes place. Then, the fraction of material leaving the system without being affected by the reaction is the probability that a particle never visits any of these regions. We now show how to compute this.

Let $A$ be a set of flow regions. For each $i \notin A$ let

$$f_A(i) = P_i\{X_1 \notin A, X_2 \notin A, \ldots\}, \tag{25}$$

be the probability that a particle which is initially in region $i$ will never enter the flow regions of $A$. Let $\mathbf{f}_A$ be a column vector whose entries are $f_A(i)$ for all $i \notin A$, and $\mathbf{Q}_A$ be the matrix obtained from $\mathbf{P}$ by deleting all rows and columns which correspond to regions of $A$. Then $\mathbf{f}_A$ is the largest solution of the system of linear equations (Cinlar, 1975)

$$\mathbf{f}_A = \mathbf{Q}_A \mathbf{f}_A, \tag{26}$$

which satisfies $1 \leq f_A(i) \leq 1$ for all $i \notin A$. The system (Eq. 26) has an infinite number of solutions which differ from each other by a constant multiplication. However,

$$f_A(r+1) = 1, \tag{27}$$

since $r+1$ is an absorbing state. Hence the new system consisting of Eqs. 26 and 27, has a unique solution.

To illustrate how this works, consider the system of Figure 2 and compute the fraction of material which never passes through Regions 4 or 7. Thus, $A = \{4,7\}$, and $\mathbf{f}_A = [f_A(1), f_A(2), f_A(3), f_A(5), f_A(6)]^T$ and the matrix $\mathbf{Q}_A$ is obtained from Eq. 5 by deleting the fourth and seventh rows and columns. Here Eqs. 26 and 27 become:

$$f_A(1) = f_A(2) \qquad f_A(5) = 3/4\, f_A(6) + 1/4\, f_A(8)$$
$$f_A(2) = 1/2\, f(3) \qquad f_A(6) = 1/8\, f_A(3) + 1/2\, f_A(6)$$
$$f_A(3) = 3/8\, f(5) \qquad f_A(8) = 1$$

and the solution is

$$f_A(1) = 0.079 \qquad f_A(5) = 0.424$$
$$f_A(2) = 0.079 \qquad f_A(6) = 0.232$$
$$f_A(3) = 0.159 \qquad f_A(8) = 1$$

The fraction of material which enters the system and avoids Regions 4 and 7, $f_A(1)$, is therefore 0.079.

## CONCLUDING REMARKS

In the foregoing analysis we have considered the movements of particles in an arbitrary system in terms of visits to flow regions in the system. In some operations particle properties or process performance may depend on the number of visits to a certain region or on the total number of regions visited (agglomeration, attrition, etc.). However, in most applications the number of visits to a region is not, in itself, a crucial process parameter. We have selected to start the analysis with the number of visits to a region, $N_j$, because it conveniently characterizes the trajectories of the particle without considering the time scale. Once $N_j$ and its distribution are known many other important process parameters can be derived as discussed in subsequent parts of this series.


## ACKNOWLEDGMENTS

Financial support for this work was made available by the Center for Energy Research, Texas Tech. University, and by the Fund for the Promotion of Research at the Technion—Israel Institute of Technology.


## NOTATIONS

$E_i[N_j]$ = expected value of $N_j$ if the initial state is $i$
$E_i[N]$ = expected value of $N$ if the initial state is $i$
$F(i,j)$ = the probability that a particle initially in $i$ will ever visit region $j$
$F_m(i)$ = the probability that a particle initially in $i$ will visit $m$ regions
$\mathbf{F}_m$ = vector whose entries are $F_m(i)$
$f_A(i)$ = the probability that a particle initially in $i$ will avoid regions in a set $A$
$\mathbf{f}_A$ = a vector whose entries are $f_A(i)$
$\mathbf{I}$ = identity matrix
$N$ = total number of regions visited
$N_j$ = number of visits to region $j$
$P(i,j)$ = transition probability from region $i$ to region $j$
$\mathbf{P}$ = matrix of transition probabilities
$p_j$ = probability of a particle passing at least once through region $j$
$q_j$ = probability that a particle initially in $j$ will never return to $j$
$R(i,j)$ = expected value of $N_j$ if the initial state is $i$
$r$ = number of transient states (or regions)
$s$ = number of absorbing states (or outlets)
$\mathrm{Var}_i[N_j]$ = variance of $N_j$, if the initial state is $i$
$X_n$ = a random variable representing the state of the Markov chain on its $n$th step

### Greek Letters

$\mu_N(j)$ = expected value of $N_j$
$\boldsymbol{\pi}$ = vector of initial probabilities $\pi(j)$
$\sigma_N^2(j)$ = variance of $N_j$
$\boldsymbol{\sigma}_N^2$ = matrix whose entires are $\mathrm{Var}_i[N_j]$

## LITERATURE CITED


Chung, K. L., "Markov Chains with Stationary Probabilities," 2nd Ed., Springer-Verlag (1967).

Çinlar, E., "Introduction to Stochastic Processes," Prentice-Hall Inc. (1975).

Feller, W., "An Introduction to Probability Theory and Its Applications," **II**, 2nd Ed., John Wiley & Sons, Inc. (1971).

Kemeny, J. G., J. L. Snell, and A. W. Knapp, "Denumerable Markov Chain," Van Nostrant (1966).

Mann, U., M. Rubinovitch, and E. J. Crosby, "Characterization and Analysis of Continuous Recycle Systems: I. Single Unit," *AICHE J.*, **25**(5), p. 873 (1979).

Mann, U., and M. Rubinovitch, "Characterization and Analysis of Continuous Recycle Systems: II. Cascade," *AICHE J.*, **27**(5), p. 829 (1981).

Schmalzer, D. K., and H. E. Hoelscher, "A Stochastic Model of Packed-Bed Mixing and Mass Transfer," *AICHE J.*, **17**(1), p. 104 (1971).

Seinfeld, J. H., and L. Lapidus, "Mathematical Methods in Chemical Engineering," Prentice-Hall (1974).

Srinivasan, S. K., and K. M. Mehta, "A Markov Chain Model for a Packed Bed," *AICHE J.*, **19**(3), p. 650 (1972).

Raghuraman, J., and V. Mohan, "A Markov Chain Model for a Packed Bed," *Chem. Eng. Sci.*, **30**, p. 549 (1975).



*Manuscript received July 21, 1981; revision received August 5, and accepted August 30, 1982.*