Mc = dimensionless magnetoconvection number after Park and Honeywell
p_{hyd} = hydrostatic pressure, N/m^2
Q = total heat transfer rate, J/s
Q_{Mg} = magnetothermal contribution to the total heat transferred due to the magnetic field gradient effect, J/s
T = temperature, °K
T_o = average T over ΔT, °K
T_1 = hot plate temperature, °K
T^* = dimensionless temperature, $T/\Delta T$
T_2 = cold plate temperature, °K
ΔT = temperature difference across the fluid, $T_1 - T_2$, °C
$\vec{u}$ = fluid velocity vector, m/s
$\vec{u}^*$ = dimensionless velocity vector, $\vec{u}D/\nu$
x^* = dimensionless coordinate, x/D

Greek Letters

α = thermal diffusivity, $\Lambda_o/\rho C_v$, m^2/s
β = coefficient of thermal expansion, $= -1/\rho\ (\partial\rho/\partial T)_p|_{T_o}$, K^{-1}
η = dynamic viscosity, Ns/m^2
η_o = average η over ΔT, Ns/m^2
Λ_o = standard thermal conductivity, W/m °K
μ = magnetic permeability
μ_o = average μ over ΔT
ν_o = average kinematic viscosity over ΔT, m^2/s
ρ = density, g/m^3
ρ_o = average ρ over ΔT, g/m^3
$\vec{\nabla}$ = del operator, m^{-1}
γ = thermal coefficient of magnetic permeability, $= -1/\mu_o\ (\partial\mu/\partial T)_p|_{T_o}$, °K^{-1}
Φ = parameter Mg/Gr

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Discrete Flow Modeling: A General Discrete Time Compartmental Model

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A general flow model is developed which is discrete both in time and space. The stirred-tank network model (continuous time compartmental model) is summarized and compared with the discrete flow model. Efficient methods for model fitting are given and demonstrated with numerical examples.

SCOPE

A new model is presented for treating data collected from multiple probes inside a stationary flow system. It is assumed that there are sufficient probes so that the state of the system is well described by the set of concentrations measured by the probes. Matrix methods are presented to relate this new model which is discrete in both time and space to the continuous time compartmental models (stirred-tank networks) commonly used in physiological modeling. The new model and the older compartmental model are both characterized by matrices of fractional input flow coefficients which give the fraction of flow coming into one region which originated in another. It is shown that the volumes of the regions can be calculated from this fractional input matrix. The fractional input matrix can also be used to find the coefficients of the linear difference equation relating the concentration in any region to its past values.

CONCLUSIONS AND SIGNIFICANCE

This paper presents a systematic method for modeling any stationary flow system. It makes use of a new model which is discrete in both time and space and compares it with the existing compartmental model which is discrete in space but continuous in time. The discrete flow model described is capable of duplicating the performance of a continuous time, discrete space flow model (stirred-tank network or compartmental model) at any set of regularly spaced times t_1, t_2, t_3 . . . . Further, there are flow systems (such as plug flow with little dispersion) which can be modeled by a low-order discrete time model but cannot be modeled with a low-order stirred-tank network. In this sense, the discrete model is more general than the compartmental model.

Continuous compartmental models are often simulated by numerical integration of a large number of differential equations. Use of the discrete model allows simulation by simple matrix multiplication. Since the discrete model can also be used to obtain exact solutions of the continuous compartment model at any regularly spaced set of time intervals, it obviates the need for numerical integration.

If multiregion transient or steady state data are available, all the parameters of the flow system can be found directly for either flow model. No search techniques are necessary. The volumes of the subregion need not be specified; it is shown that they can be calculated from the other system parameters.

Modeling flow between different regions in a system is important in engineering applications. For instance, the performance of a chemical reactor can only be predicted if the flow patterns within the system are known; the effectiveness (or toxicity) of a drug in the body can only be understood if it is known how the drug moves from region to region or organ to organ in the body. The movement of groundwater is an important variable in water quality studies. Many more examples can be found.

The approaches that have been used in modeling flow (and mixing) can be divided into two broad categories; the first treats both time and space as continuous variables. The resulting partial differential equations describing flow contain both diffusion and convection terms. Application is limited to regions of known size and shape, and closed form solutions are obtained only for simple geometries. In the second approach, space is treated as a discrete variable; compartments are used, and ordinary differential equations describe flow into and out of the compartments. The mixing effect of diffusion is accounted for by assuming that each compartment is well mixed and that the scale of mixing determines the size of these compartments. Flow streams between compartments include the combined effects of convection and diffusion. The latter approach has been described in the literature by Buffham et al. (1969) and by Wen and Fan (1975) and has been developed and used extensively in physiology to describe flow within an organism (for instance, Rubinow, 1975).

A third approach is possible in which both time and space are discrete. It is more general, and it is computationally simpler than the continuous time compartment model and it agrees precisely with the continuous time compartmental model at regularly spaced discrete values of time. It is this approach which is developed in this paper.

THE DISCRETE TIME COMPARTMENTAL MODEL

The model assumes that the behavior of a given flow system can be represented by n regions which are connected by an arbitrary flow network as shown in Figure 1. The flows are discrete in time rather than continuous. The volumes of the regions are not necessarily equal.

In order to visualize a physical process which corresponds to the mathematical model, consider each region to contain a piston which moves from the top of the region down to the bottom in one transition. During a transition, all the material below each piston is displaced, either back into the top chamber of the same region, into the top chambers of other regions, or else into the exit station. As the streams enter a region, they mix completely with each other so that the composition in each region is uniform.

The same process is repeated for the next transition. Consider a system at some time t after a tracer has been introduced. The state of the system is described by the tracer concentration in each of the n regions. Let the time interval for one transition be Δt. Then, from the mass balance of the tracer around the j^{th} region at time $t + \Delta t$, we find

$$V_j c_j(t + \Delta t) = \sum_{i=1}^{n} (q_{ij}\Delta t)\, c_i(t) + (q_{\text{in},j}\Delta t) f_j(t), \quad \text{for all } t \geq 0 \quad j = 1, 2, \ldots n \qquad (1)$$

where $c_j(t + \Delta t)$ is the tracer concentration in region j at time $t + \Delta t$, $c_i(t)$ is the tracer concentration in region i at time t, and $f_j(t)$ is the input tracer concentration from the feed station to region j at time t. Defining

$$p_{ij} = \frac{q_{ij}\Delta t}{V_j} \qquad i, j = 1, 2, \ldots n \qquad (2)$$

and

$$p_{\text{in},j} = \frac{q_{\text{in},j}\Delta t}{V_j} \qquad j = 1, 2, \ldots n \qquad (3)$$

we get

$$c_j(t + \Delta t) = \sum_{i=1}^{n} p_{ij} c_i(t) + p_{\text{in},j} f(t) \quad j = 1, 2, \ldots n \qquad (4a)$$

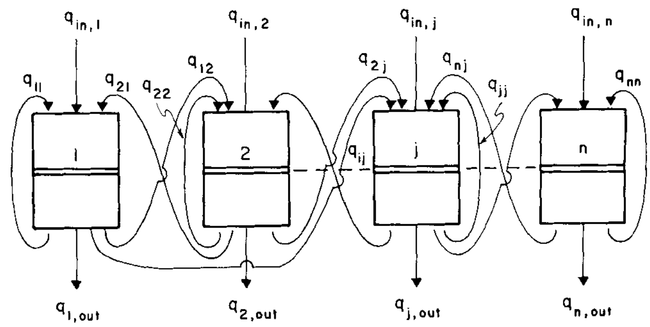

Fig. 1. Diagram of the discrete time compartmental model.

where p_{ij} is called the fractional input coefficient, and $p_{in,j}$ is the feed coefficient. In general

$$c_j[t + (m+1)\Delta t] = \sum_{i=1}^{n} p_{ij} c_i(t + m\Delta t) + p_{in,j} f(t) f_j(t + m\Delta t), \quad j = 1, 2, \ldots n, \quad m = 0, 1, 2, \ldots \tag{4b}$$

The above equation can be written in matrix notation as

$$\mathbf{C}(m+1) = \mathbf{C}(m)\mathbf{P} + \mathbf{F}(m)\mathbf{P}_{in} \quad m = 0, 1, 2 \ldots \tag{5}$$

where $\mathbf{C}(m)$ is the concentration row vector at time $m\Delta t$

$$\mathbf{C}(m) = [c_1(m) \;\; c_2(m) \;\; \ldots \;\; c_n(m)]$$

$\mathbf{F}(m)$ is the input concentration row vector at time $m\Delta t$

$$\mathbf{F}(m) = [f_1(m) \;\; f_2(m) \;\; \ldots \;\; f_n(m)]$$

$\mathbf{P}$ is the fractional input matrix of the flow system with elements p_{ij}, that is

$$\mathbf{P} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \cdot & \cdot & & \\ \cdot & \cdot & & \\ \cdot & \cdot & & \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{bmatrix}$$

and $\mathbf{P}_{in}$ is the feed matrix with diagonal elements $p_{in,j}$, that is

$$\mathbf{P}_{in} = \begin{bmatrix} p_{in,1} & 0 & \cdots & 0 \\ 0 & p_{in,2} & \cdots & 0 \\ & & \ddots & \\ 0 & 0 & \cdots & p_{in,n} \end{bmatrix}$$

If no tracer is introduced for $t \geqq 0$, the input tracer concentration row vector $\mathbf{F}(m)$ becomes zero for $m \geqq 0$. Then, Equation (5) becomes

$$\mathbf{C}(m+1) = \mathbf{C}(m)\mathbf{P}, \quad m = 0, 1, 2 \ldots \tag{6}$$

Since by recursion

$$\mathbf{C}(1) = \mathbf{C}(0)\mathbf{P}$$

$$\mathbf{C}(2) = \mathbf{C}(1)\mathbf{P} = \mathbf{C}(0)\mathbf{P}^2$$

$$\mathbf{C}(3) = \mathbf{C}(2)\mathbf{P} = \mathbf{C}(0)\mathbf{P}^3$$

in general

$$\mathbf{C}(m) = \mathbf{C}(0)\mathbf{P}^m \quad m = 0, 1, 2, \ldots \tag{7}$$

From this equation the tracer in any cell at time $m = 1, 2, \ldots$ can be calculated directly by matrix multiplication.

All the fractional input coefficients p_{ij} in the fractional input matrix must be non-negative and not greater than 1. The sum over the j^{th} column is

$$\sum_{i=1}^{n} p_{ij} = \frac{\sum_{i=1}^{n} q_{ij}}{V_j}$$

It follows that this sum will be 1 if there is no inlet to the j^{th} region from the inlet station. If the j^{th} region has an inlet then the sum will be less than 1. Because the volumes of the regions are not generally equal, no such simple relation holds for the sum of the p_{ij} in the i^{th} row.

USE OF THE FRACTIONAL INPUT MATRIX

Computing the Volumes of the Regions

From Equation (2), we know

$$p_{ij} = \frac{q_{ij}\Delta t}{V_j} \quad i, j = 1, 2, \ldots n$$

Thus

$$p_{ij} V_j = q_{ij}\Delta t \quad i, j = 1, 2, \ldots n$$

or

$$\sum_{i=1}^{n} p_{ij} V_j = \sum_{j=1}^{n} q_{ij}\Delta t \quad i = 1, 2, \ldots, n \tag{8}$$

Case 1. If region i has no outlet to the outlet station, then

$$\sum_{j=1}^{n} q_{ij}\Delta t = V_i \quad i = 1, 2, \ldots n \tag{9}$$

Substituting Equation (9) into Equation (8), we get

$$\sum_{j=1}^{n} p_{ij} V_j = V_i \quad i = 1, 2, \ldots n \tag{10}$$

Case 2. If region i has an outlet to the outlet station, then

$$\sum_{j=1}^{n} q_{ij}\Delta t = V_i - (q_{i,out}\Delta t) \quad i = 1, 2, \ldots n \tag{11}$$

Substituting Equation (11) into Equation (8), we get

$$\sum_{j=1}^{n} p_{ij} V_j = V_i - (q_{i,out}\Delta t) \quad i = 1, 2, \ldots n \tag{12}$$

Now suppose that a flow system of n regions has some outlets to the outlet station, say from region k and region n for example. Then Equations (10) and (12) can be written together in matrix form as

$$\mathbf{P} \cdot \mathbf{V} = \mathbf{V} - \mathbf{Q}_{out}\Delta t \tag{13}$$

where $\mathbf{V}$ and $\mathbf{Q}_{out}$ are the column vectors

$$\mathbf{V} = \begin{bmatrix} V_1 \\ V_2 \\ \cdot \\ \cdot \\ \cdot \\ V_n \end{bmatrix}; \quad \mathbf{Q}_{out} = \begin{bmatrix} q_{1,out} \\ q_{2,out} \\ \cdot \\ \cdot \\ \cdot \\ q_{n,out} \end{bmatrix} \tag{14}$$

Thus

$$(\mathbf{P} - \mathbf{I}) \cdot \mathbf{V} = -\mathbf{Q}_{out} \tag{15}$$

If $(\mathbf{P} - \mathbf{I})$ is nonsingular, the matrix $(\mathbf{P} - \mathbf{I})$ is invertible, and the volumes can be found from the relationship

$$\mathbf{V} = (\mathbf{I} - \mathbf{P})^{-1} \cdot \mathbf{Q}_{out} \tag{16}$$

If there are no outlets from this system, $(\mathbf{P} - \mathbf{I})$ becomes singular, and Equation (16) cannot be used to calculate regional volumes. If the total volume of the system is to remain constant, there cannot be any input streams either; hence each column in the $\mathbf{P}$ matrix will sum to 1. In this case, we may eliminate a row from the $\mathbf{p}$ matrix without losing any information. For instance, we may write

$$\begin{bmatrix} V_1 \\ V_2 \\ \cdot \\ \cdot \\ \cdot \\ V_{n-1} \end{bmatrix} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ & & & \\ p_{n-1,1} & p_{n-1,2} & \cdots & p_{n-1,n} \end{bmatrix} \cdot \begin{bmatrix} V_1 \\ V_2 \\ \cdot \\ \cdot \\ \cdot \\ V_{n-1} \end{bmatrix} \tag{17}$$

or, more compactly

$$\tilde{\mathbf{V}} = \tilde{\mathbf{p}} \cdot \tilde{\mathbf{V}}$$

Now, by adding the equation

$$\mathbf{V}_T + \mathbf{V}_n = \mathbf{V}_1 + \mathbf{V}_2 + \mathbf{V}_3 + \ldots + 2\mathbf{V}_n$$

as the last row, we obtain

$$\begin{bmatrix} [\tilde{\mathbf{V}}] \\ [\mathbf{V}_T + \mathbf{V}_n] \end{bmatrix} = \begin{bmatrix} [\tilde{p}] \\ [1 \ \ 1 \ \ldots \ 2] \end{bmatrix} \cdot \mathbf{V} \quad (18)$$

Since

$$\begin{bmatrix} [\tilde{\mathbf{V}}] \\ [\mathbf{V}_T + \mathbf{V}_n] \end{bmatrix} = \mathbf{V} + \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \mathbf{V}_T \end{bmatrix}$$

it follows that

$$\begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{V}_T \end{bmatrix} = \begin{bmatrix} [\tilde{\mathbf{p}}] \\ [1 \ \ 1 \ldots 1] \end{bmatrix} \cdot \mathbf{V} \quad (19)$$

and thus the volumes can be found by inversion:

$$\mathbf{V} = \begin{bmatrix} [\tilde{\mathbf{p}}] \\ [1 \ \ 1 \ldots 1] \end{bmatrix}^{-1} \cdot \begin{bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{V}_T \end{bmatrix} \quad (20)$$

Age Distribution in the Flow Systems

The **I** curves (internal age distributions) for each region and the **F** curve of the flow system can be calculated from the fractional input matrix **P**. For simplicity, assume that all the material enters the system from a single inlet station and all leaves into a single outlet station.

Suppose that a flow system consists of n regions. In order to compute the **I** curves and the **F** curve simultaneously, we include an accumulating outlet station designated by the subscript $n+1$. The augmented fractional input matrix **P** is written as

$$\overline{\mathbf{P}} = \begin{bmatrix} p_{11} & p_{12} & \cdot\cdot & p_{1n} & p_{1,n+1} \\ p_{21} & p_{22} & \cdot\cdot & p_{2n} & p_{2,n+1} \\ \cdot & \cdot & & \cdot & \cdot \\ \cdot & \cdot & & \cdot & \cdot \\ p_{n1} & p_{n2} & \cdot\cdot & p_{nn} & p_{n,n+1} \\ p_{n+1,1} & p_{n+1,2} & \cdot\cdot & p_{n+1,n} & p_{n+1,n+1} \end{bmatrix}$$

Once the tracer enters the accumulating outlet station, it stays there permanently; hence

$$p_{n+1,i} = \begin{Bmatrix} 0 & i \neq n+1 \\ 1 & i = n+1 \end{Bmatrix} \quad (21)$$

Thus, the last row of $\overline{\mathbf{p}}$ becomes

$$[0 \ \ 0 \ \ . \ . \ . \ \ 0 \ \ 1]$$

If no tracer is introduced for $t \geqq 0$, we may write [analogous to Equation (7)]

$$\overline{\mathbf{C}}(m) = \overline{\mathbf{C}}(0)\overline{\mathbf{P}}^m \qquad m = 0, 1, 2, \ldots \quad (22)$$

where $\overline{\mathbf{C}}(0)$ is tracer concentration row vector including the outlet station at $t = 0$, and $\overline{\mathbf{C}}(m)$ is tracer concentration row vector including the outlet station at $t = m\Delta t$.

Suppose that we inject a unit of tracer into the inlet station at $t = 0$; then $c_1(m)$, $c_2(m)$, . . ., and $c_n(m)$, $m = 0, 1, 2, \ldots$ computed by Equation (22) are the internal age distributions (**I** curves) for region 1, region 2, . . ., and region n of the flow system. $c_{n+1}(m)$, $m = 0, 1, 2, \ldots$ computed by Equation (22) is the F curve or step response of the system. The E curve or system residence time distribution can be obtained by differencing the F curve.

Calculation of Steady State Responses

Consider a flow system which is assumed to consist of n regions as shown in Figure 1. Suppose the initial state is zero

$$\mathbf{C}(0) = [0 \ \ 0 \ \ . \ \ . \ \ 0]$$

and there is a steady tracer inlet to region 1 (only) given by

$$\mathbf{F}(m) = \left[\frac{1}{p_{\text{in},1}} \ 0 \ldots 0\right], \qquad m = 0, 1, 2, \ldots$$

Then, the inlet row vector is

$$\mathbf{F}(m)\mathbf{P}_{\text{in}} = \left[\frac{1}{p_{\text{in},1}} 0 \ldots 0\right] \cdot \begin{bmatrix} p_{\text{in},1} & 0 & \ldots & 0 \\ 0 & p_{\text{in},2} & \ldots & 0 \\ & & \cdot & \\ & & \cdot & \\ & & \cdot & \\ 0 & 0 & \ldots & p_{\text{in},n} \end{bmatrix}$$

$$= [1 \ \ 0 \ . \ . \ . \ 0]$$

Substituting into Equation (13), we find

$$\mathbf{C}(1) = \mathbf{C}(0)\mathbf{P} + \mathbf{F}(0)\mathbf{P}_{\text{in}} = [0 \ 0 \ldots 0] + [1 \ 0 \ldots 0] = [1 \ 0 \ldots 0]$$

$$\mathbf{C}(2) = \mathbf{C}(1)\mathbf{P} + \mathbf{F}(1)\mathbf{P}_{\text{in}} = [1 \ 0 \ldots 0]\,\mathbf{P} + [1 0 \ldots 0]$$

$$\mathbf{C}(3) = \mathbf{C}(2)\mathbf{P} + \mathbf{F}(2)\mathbf{P}_{\text{in}} = [1 \ 0 \ldots 0]\,\mathbf{P}^2 + [1 \ 0 \ldots 0]\,\mathbf{P} + [1 \ 0 \ldots 0]$$

In general

$$\mathbf{C}(m+1) = [1 \ 0 \ldots 0]\,\mathbf{P}^m + [1 \ 0 \ldots 0]\,\mathbf{P}^{m-1} + \ldots + [1 \ 0 \ldots 0]\,\mathbf{P} + [1 \ 0 \ldots 0]$$
$$= [1 \ 0 \ldots 0]\,(\mathbf{P}^m + \mathbf{P}^{m-1} + \ldots + \mathbf{P} + \mathbf{I}) \quad (23)$$

We define the limit as $m \to \infty$ as

$$\lim_{m\to\infty} \mathbf{C}(m+1) = [s_{11} \ s_{12} \ \ . \ . \ \ s_{1n}] \quad (24)$$

Here s_{ij} is the steady response at region j to a steady input at region i. It is the concentration that would occur at j if tracer is constantly injected into region i such that the concentration in i is s_{ii}. Substituting Equation (24) into Equation (23), we obtain

$$[s_{11} \ s_{12} \ldots s_{1n}] = [1 \ 0 \ldots 0] \cdot \lim_{m\to\infty} (\mathbf{P}^m + \mathbf{P}^{m-1} + \ldots + \mathbf{P} + \mathbf{I})$$

Since

$$\lim_{m\to\infty} (\mathbf{P}^m + \mathbf{P}^{m-1} + \ldots + \mathbf{P} + \mathbf{I}) = (\mathbf{I} - \mathbf{P})^{-1}$$

Equation (25) becomes

$$[s_{11} \ s_{12} \ldots s_{1n}] = [1 \ 0 \ldots 0]\,(\mathbf{I} - \mathbf{P})^{-1} \quad (26)$$

Similarly

$$[s_{21}\ s_{22}\ \dots\ s_{2n}] = [0\ 1\ \dots\ 0]\ (\mathbf{I}-\mathbf{P})^{-1}$$
$$\vdots \qquad\qquad \vdots$$
$$[s_{n1}\ s_{n2}\ \dots\ s_{nn}] = [0\ 0\ \dots\ 1]\ (\mathbf{I}-\mathbf{P})^{-1} \tag{27}$$

Combining Equations (26) and (27), we obtain

$$\begin{bmatrix} s_{11} & s_{12} & \dots & s_{1n} \\ s_{21} & s_{22} & \dots & s_{2n} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ s_{n1} & s_{n2} & \dots & s_{nn} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & \dots & 1 \end{bmatrix} = (\mathbf{I}-\mathbf{P})^{-1} \tag{28}$$

or simply

$$\mathbf{S} = (\mathbf{I}-\mathbf{P})^{-1} \tag{29}$$

Computing Transient Concentrations from Different Equations

For a flow system with n regions, the Cayley-Hamilton theorem states that the matrix $\mathbf{P}$ must satisfy an n^{th} order equation

$$\mathbf{P}^n + \alpha_{n-1}\mathbf{P}^{n-1} + \dots + \alpha_1\mathbf{P} + \alpha_0\mathbf{I} = 0 \tag{30}$$

where the α_i's are constants, obtained by setting $\text{Det}(\mathbf{P} - \lambda\mathbf{I}) = 0$; that is

$$\text{Det}(\mathbf{P} - \lambda\mathbf{I}) = \lambda^n + \alpha_{n-1}\lambda^{n-1} + \dots + \alpha_0 = 0$$

Multiplying by $\mathbf{C}(0)$ on both sides of Equation (30), we obtain

$$\mathbf{C}(0)\ (\mathbf{P}^n + \alpha_{n-1}\mathbf{P}^{n-1} + \dots + \alpha_1\mathbf{P} + \alpha_0\mathbf{I}) = 0 \tag{31a}$$

If there is no tracer input for $t \geqq 0$, this becomes

$$\mathbf{C}(n) + \alpha_{n-1}\mathbf{C}(n-1) + \dots + \alpha_1\mathbf{C}(1) + \alpha_0\mathbf{C}(0) = 0 \tag{31b}$$

Equation (31*b*) states that during the tracer washout each region satisfies the difference equation

$$c_i(n) + \alpha_{n-1}c_i(n-1) + \dots + \alpha_1 c_i(1) + \alpha_0 c_i(0) = 0 \tag{32}$$

COMPARISON OF DISCRETE TIME COMPARTMENTAL MODEL AND STIRRED-TANK NETWORK MODEL

The stirred-tank network model shown in Figure 2 assumes that the behavior of a flow system can be represented by n stirred tanks which are connected by an arbitrary flow network. The volumes of the tanks are not necessarily equal. Denote the volume of the i^{th} tank by V_i' and the volumetric flow rate from the i^{th} tank to the j^{th} tank by q'. The volumetric flow rate from the inlet station (or feed station) to the j^{th} tank is denoted by $q_{\text{in},j}$ and the volumetric flow rate from the i^{th} tank to the outlet station is $q_{i,\text{out}}$.

Suppose that we inject a pulse of tracer into a flow system as is shown in Figure 2. The mass balance for the tracer in the j^{th} tank gives

$$V_j'\frac{dc_j(t)}{dt} = \left[-\sum_{\substack{i=1\\i\neq j}}^{n} q'_{ji}\right] c_j(t) + \sum_{\substack{i=1\\i\neq j}}^{n} q'_{ij}c_i(t) - q'_{j,\text{out}}c_j(t) + q'_{\text{in},j}f_j(t) \qquad j = 1, 2, \dots n \tag{33}$$

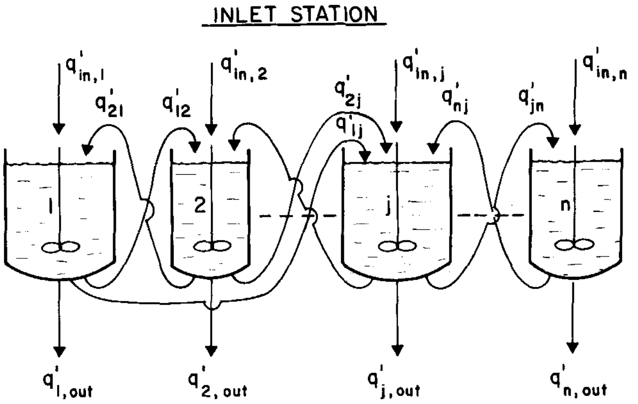

Fig. 2. Diagram of the continuous time compartmental model (stirred-tank network).

where $c_j(t)$ is the tracer concentration in the tank j at time t, and $f_j(t)$ is the tracer concentration in the stream from the inlet station to compartment j. Define

$$q'_{jj} = -\sum_{\substack{i=1\\i\neq j}}^{n} q'_{ji} - q'_{j,\text{out}} \qquad j = 1, 2, \dots n \tag{34}$$

This notation makes the matrix more compact. But note that q'_{jj} does not denote a self-flow from j to j but rather the negative of the total flow out of j. Then

$$V_j'\frac{dc_j(t)}{dt} = \sum_{i=1}^{n} q'_{ij}c_i(t) + q'_{\text{in},j}f_j(t) \qquad \text{for all } t \geqq 0,\ j = 1, 2, \dots n \tag{35}$$

Dividing by V_j' on both sides of Equation (35) and defining

$$r_{ij} = \frac{q'_{ij}}{V_j'} \qquad i, j = 1, 2, \dots n \tag{36}$$

we get

$$\frac{dc_j(t)}{dt} = \sum_{i=1}^{n} r_{ij}c_i(t) - r_{\text{in},j}f(t) \qquad j = 1, 2, \dots n \tag{37}$$

where the fractional input coefficient r_{ij} is the fraction of the flow entering tank j from tank i.

The above equation can be written in matrix notation as

$$\frac{d\mathbf{C}(t)}{dt} = \mathbf{C}(t)\mathbf{R} + \mathbf{F}(t)\mathbf{R}_{\text{in}} \qquad \text{for all } t \geqq 0 \tag{38}$$

where $\mathbf{C}(t)$ is the tracer concentration row vector with elements $c_i(t)$, $\mathbf{F}(t)$ is the tracer concentration row vector with elements $f_i(t)$, $\mathbf{R}$ is the fraction input matrix with elements r_{ij}, that is

$$\mathbf{R} = \begin{bmatrix} r_{11} & r_{12} & \dots & r_{1n} \\ r_{21} & r_{22} & \dots & r_{2n} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ r_{n1} & r_{n2} & \dots & r_{nn} \end{bmatrix},$$

and $\mathbf{R}_{\text{in}}$ is the feed matrix with diagonal elements $r_{\text{in},j}$, that is

$$\mathbf{R}_{\text{in}} = \begin{bmatrix} r_{\text{in},1} & 0 & \dots & 0 \\ 0 & r_{\text{in},2} & \dots & 0 \\ & & \cdot & \\ & & & \cdot \\ & & & \cdot \\ 0 & 0 & \dots & r_{\text{in},n} \end{bmatrix}$$

For a given set of initial conditions $\mathbf{C}(0)$ and no tracer flow into the system, the general solution of Equation (38) is

$$\mathbf{C}(t) = \mathbf{C}(0)\exp(\mathbf{R}t) \qquad \text{for all } t \geqq 0 \tag{39}$$

where the matrix $\exp(\mathbf{R})$ is defined as

$$\mathbf{I} + \frac{\mathbf{R}}{1!} + \frac{\mathbf{R}^2}{2!} + \frac{\mathbf{R}^3}{3!} + \ldots .$$

Relation Between Matrices P and R

Suppose that we would like to find a matrix R for a stirred-tank network model (continuous time process) that will have the same tracer concentration as the discrete flow model (discrete time process) described by the matrix $\mathbf{P}$ at $t = 0, \Delta t, 2\Delta t, \ldots$. Comparing Equations (39) and (7) when $t = m\Delta t$, we find

$$\exp(\mathbf{R}\Delta t) = \mathbf{P} \tag{40}$$

or

$$\mathbf{R} = \frac{\ln\mathbf{P}}{\Delta t} \tag{41}$$

The matrix $\mathbf{P}$ for the discrete time compartmental model and the matrix $(\mathbf{I} + \mathbf{R}\Delta t)$ for stirred-tank network model are nearly identical if Δt is sufficiently small and if $\ln p$ converges. For every stirred-tank network model, we can find the corresponding discrete flow model according to Equation (40). This is not true in the other direction, since the convergence of $\ln p$ depends on the eigenvalues λ of matrix $\mathbf{P}$. In this sense the discrete flow model is more general than stirred-tank network model.

Relation Between V_{discrete} and $V_{\text{continuous}}$

From the definition of r_{ij} [Equation (36)], we know

$$\mathbf{R}\cdot\begin{bmatrix} \mathbf{V}_1' \\ \mathbf{V}_2' \\ \cdot \\ \cdot \\ \cdot \\ {}_n\mathbf{V}' \end{bmatrix}_{\text{continuous}} = \begin{bmatrix} -q'_{1,\text{out}} \\ -q'_{2,\text{out}} \\ \cdot \\ \cdot \\ \cdot \\ -q'_{n,\text{out}} \end{bmatrix} \tag{42}$$

or simply

$$\mathbf{R}\cdot\mathbf{V}' = \mathbf{Q}'_{\text{out}}$$

If matrix $(\mathbf{R})$ is nonsingular, then the compartmental volumes for the continuous time model are obtained from

$$\mathbf{V}' = -\mathbf{R}^{-1}\cdot\mathbf{Q}'_{\text{out}} \tag{43}$$

Now, if we substitute Equation (41) into Equation (43) and then compare it with Equation (16), we find

$$\mathbf{V}' = [\ln\mathbf{P}]^{-1}\cdot[\mathbf{P}-\mathbf{I}]\cdot\mathbf{V} \tag{44}$$

Similarly

$$\mathbf{V} = \frac{\exp[\mathbf{R}\Delta t]}{\Delta t}\mathbf{R}\cdot\mathbf{V}' \tag{45}$$

Equations (44) and (45) give the relationships between the volumes of the regions for discrete flow model and the volumes of the tanks for stirred-tank network model. If $\Delta t \to 0$, then $\mathbf{V}_{\text{discrete}}$ will be equal to $\mathbf{V}'$.

FITTING THE DISCRETE TIME COMPARTMENTAL MODEL TO REAL DATA

Steady State Data

The fractional input coefficients p_{ij} can be obtained from steady state tracer data using Equation (29). For a model with n regions, a steady tracer signal is injected into each of the n regions, and the resulting tracer concentrations is measured in each of the n regions. In all, n^2 measurements are needed, corresponding to the n^2 elements in the $\mathbf{S}$ matrix. The $\mathbf{P}$ matrix is then found by the relation

$$\mathbf{P} = \mathbf{I} - \mathbf{S}^{-1} \tag{46}$$

Transient Data

The $\mathbf{P}$ matrix can also be obtained from transient data. For a model with n regions, the required data consist of $(n + 1)$ transient concentration readings for each of the n regions. This can be shown as follows.

Consider a flow system which consists of n regions. For a pulse tracer input at $t = 0$, the state transition equation of the discrete flow model becomes

$$\mathbf{C}(m) = \mathbf{C}(0)\mathbf{P}^m \qquad m = 0, 1, 2, \ldots \tag{7}$$

Thus

$$\begin{aligned} \mathbf{C}(1) &= \mathbf{C}(0)\mathbf{P} \\ \mathbf{C}(2) &= \mathbf{C}(0)\mathbf{P}^2 = \mathbf{C}(1)\mathbf{P} \\ \mathbf{C}(3) &= \mathbf{C}(0)\mathbf{P}^3 = \mathbf{C}(2)\mathbf{P} \\ &\;\;\vdots \\ \mathbf{C}(n-1 &= \mathbf{C}(0)\mathbf{P}^{n-1} = \mathbf{C}(n-2)\mathbf{P} \\ \mathbf{C}(n) &= \mathbf{C}(0)\mathbf{P}^n = \mathbf{C}(n-1)\mathbf{P} \end{aligned} \tag{47}$$

Equation (47) can be written as

$$\begin{bmatrix} \mathbf{C}(1) \\ \mathbf{C}(2) \\ \mathbf{C}(3) \\ \cdot \\ \cdot \\ \mathbf{C}(n-1) \\ \mathbf{C}(n) \end{bmatrix} = \begin{bmatrix} \mathbf{C}(0) \\ \mathbf{C}(1) \\ \mathbf{C}(2) \\ \cdot \\ \cdot \\ \mathbf{C}(n-2) \\ \mathbf{C}(n-1) \end{bmatrix}\cdot\mathbf{P} \tag{48}$$

or more briefly

$$[\mathbf{C}_{t+1}] = [\mathbf{C}_t]\cdot\mathbf{P}$$

If the first square matrix in the right-hand side of Equation (48) is nonsingular, then the unique solution of Equation (48) is

$$\mathbf{P} = [\mathbf{C}_t]^{-1}\cdot[\mathbf{C}_{t+1}] \tag{49}$$

Thus, in order to find the fractional input matrix $\mathbf{P}$ for a pulse tracer input, the only information needed is $(n + 1)$ successive transient tracer measurements for each of the n regions.

Transient Data with Redundancy

We now consider what is the best way to find the $\mathbf{P}$ matrix if extra data are available; say, for instance, that we have transient tracer concentrations measured at $m > n + 1$ points in time. Then

$$\begin{bmatrix} \mathbf{C}(1) \\ \mathbf{C}(2) \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{C}(m) \end{bmatrix} = \begin{bmatrix} \mathbf{C}(0) \\ \mathbf{C}(1) \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{C}(m-1) \end{bmatrix}\cdot\mathbf{P} \tag{50}$$

Consider only the j^{th} column in the left-hand matrix:

$$\begin{bmatrix} C_j(1) \\ C_j(2) \\ C_j(3) \\ C_j(m) \end{bmatrix} = \begin{bmatrix} C_1(0) & C_2(0) & \ldots & C_n(0) \\ C_1(1) & C_2(1) & \ldots & C_n(1) \\ \ldots & \ldots & \ldots & \ldots \\ C_1(m-1) & C_2(m-1) & \ldots & C_n(m-1) \end{bmatrix}\cdot\begin{bmatrix} p_{j1} \\ p_{j2} \\ p_{j3} \\ p_{jn} \end{bmatrix} \tag{51}$$

This equation holds exactly for the model but of course is only an approximation for real data. The left-hand side represents the actual tracer measurements at region j, and the right-hand side represents the values predicted by the model. We would like to find the column vector

$$\begin{bmatrix} p_{j1} \\ p_{j2} \\ \cdot \\ \cdot \\ \cdot \\ p_{jn} \end{bmatrix}$$

which minimizes the discrepancy. We do this by minimizing the sum of the squares of the errors. Rewrite Equation (51) in the form

$$y = Wx \tag{52}$$

Then

$$\Sigma(y - Wx)^2 = (y - Wx)^T(y - Wx) \tag{53}$$

Setting the derivative with respect to each element in x equal to zero, we get

$$-2(y^tW - x^TW^TW) = 0$$

Thus

$$x = (W^TW)^{-1}(W^Ty) \tag{54}$$

Since y is any column in the matrix

$$\begin{bmatrix} \mathbf{C}(1) \\ \mathbf{C}(2) \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{C}(m) \end{bmatrix}$$

and x is the corresponding column in n the $\mathbf{P}$ matrix, it follows that the error between predicted and measured values is minimized where the $\mathbf{P}$ matrix is found according to the formula

$$\mathbf{P} = \left[\begin{bmatrix} \mathbf{C}(0) \\ \mathbf{C}(1) \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{C}(m-1) \end{bmatrix}^T \cdot \begin{bmatrix} \mathbf{C}(0) \\ \mathbf{C}(1) \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{C}(m-1) \end{bmatrix} \right]^{-1} \cdot \left[\begin{bmatrix} \mathbf{C}(0) \\ \mathbf{C}(1) \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{C}(m-1) \end{bmatrix}^T \cdot \begin{bmatrix} \mathbf{C}(1) \\ \mathbf{C}(2) \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{C}(m) \end{bmatrix} \right] \tag{55}$$

A NUMERICAL EXAMPLE

We now show how the discrete time compartmental model can be used to represent a flow system.

For this purpose we have generated a table of data representing tracer concentrations as a function of time at twenty-five points inside a hypothetical flow system. The data are simulated to represent a flow process with mixing caused by both velocity gradients and diffusion. The model used to generate the data is shown in Figure 3. Each of the twenty-five cells has a volume of 1. The numbers shown on arrows between the cells represent the volumetric flow between regions in an amount of time $\Delta t = 1$ s. For example, for region 1

$$\begin{aligned} q_{in,1} &= 0.15 \text{ l/s} \\ q_{12} &= 0.2 \text{ l/s} \\ q_{21} &= 0.05 \text{ l/s} \\ &\text{etc.} \end{aligned}$$

At time 0, tracer is introduced into the five cells at the left, so that at $t = 0$

$$\begin{aligned} c(1) &= 0.3 \\ c(6) &= 0.2 \\ c(11) &= 0.2 \\ c(16) &= 0.2 \\ c(21) &= 0.1 \end{aligned}$$

The tracer input is biased (as it would likely be in a real experiment); more tracer enters region 1 and less tracer enters region 21 than ought to enter.

Now suppose we wished to model this system with data measured only at three points inside the system, namely, in regions 11, 13, and 15. The data record for these points is given in Table 1. We select data taken at 8 s intervals beginning at $t = 10$ (to allow the tracer to disperse a bit through the system. This gives

$$\begin{aligned} t = 10 \quad \mathbf{C}(0) &= [0.0372 \quad 0.0546 \quad 0.0159] \\ t = 18 \quad \mathbf{C}(1) &= [0.0142 \quad 0.0427 \quad 0.0383] \\ t = 26 \quad \mathbf{C}(2) &= [0.0062 \quad 0.0258 \quad 0.0379] \\ t = 34 \quad \mathbf{C}(3) &= [0.0029 \quad 0.0147 \quad 0.0279] \end{aligned}$$

Substituting these values into Equation (50), we find

$$\mathbf{P} = \begin{bmatrix} 0.0372 & 0.0546 & 0.0159 \\ 0.0142 & 0.0427 & 0.0383 \\ 0.0062 & 0.0258 & 0.0379 \end{bmatrix}^{-1} \cdot \begin{bmatrix} 0.0142 & 0.0427 & 0.0383 \\ 0.0062 & 0.0258 & 0.0379 \\ 0.0029 & 0.0147 & 0.0279 \end{bmatrix}$$

$$\mathbf{P} = \begin{bmatrix} 0.3192 & 0.5630 & 0.0761 \\ 0.0443 & 0.3896 & 0.5474 \\ 0.0000 & 0.0306 & 0.3511 \end{bmatrix}$$

Inlet Location

We now use this matrix to see which region has an inlet:

$$\sum_{(i)} p_{i1} = 0.3192 + 0.0443 + 0 = 0.3635 < 1$$

$$\sum_{(i)} p_{i2} = 0.5630 + 0.3896 + 0.0306 = 0.9832 \cong 1$$

$$\sum_{(i)} p_{i3} = 0.0761 + 0.5474 + 0.3511 = 0.9746 \cong 1$$

The first sum is less than 1; thus the model correctly finds that region 1 has an inlet from the inlet station.

Prediction Based on Model

We now use the calculated 3 × 3P matrix and Equation (5) to predict the concentration at $t = 42$ ($m = 4$):

$$[\mathbf{C}_1(4)\ \mathbf{C}_2(4)\ \mathbf{C}_3(4)] = [0.0029 \quad 0.0147 \quad 0.0279] \begin{bmatrix} 0.3192 & 0.5630 & 0.0761 \\ 0.0443 & 0.3896 & 0.5474 \\ 0.0000 & 0.0306 & 0.3511 \end{bmatrix}$$

$$[\mathbf{C}_1(4)\ \mathbf{C}_2(4)\ \mathbf{C}_3(4)] = [0.0016 \quad 0.0082 \quad 0.0181]$$

From Table 1 we see that the agreement is good; at $t = 42$, the correct concentrations are

$$[0.0014 \quad 0.0083 \quad 0.0182]$$

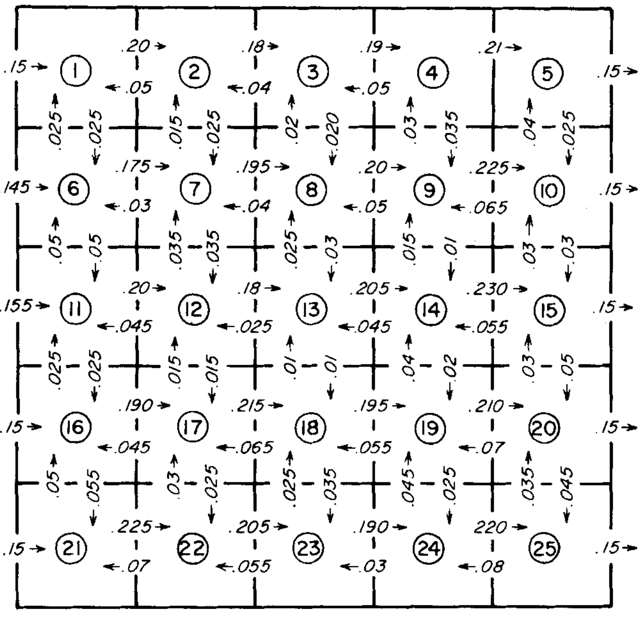

Fig. 3. Simulated flow system used to generate data for the numerical example.

TABLE 1. TRACER DATA FOR CELLS 11, 13, AND 15 IN THE SIMULATED FLOW SYSTEM OF FIGURE 3

Time (s)	Cell 11	Cell 13	Cell 15
0	0.2000	0.0000	0.0000
2	0.1316	0.0072	0.0000
4	0.0913	0.0267	0.0003
6	0.0659	0.0423	0.0030
8	0.0490	0.0513	0.0086
10	0.0372	0.0546	0.0159
12	0.0288	0.0542	0.0234
14	0.0225	0.0514	0.0300
16	0.0178	0.0473	0.0350
18	0.0142	0.0427	0.0383
20	0.0115	0.0381	0.0400
22	0.0093	0.0337	0.0403
24	0.0076	0.0296	0.0395
26	0.0062	0.0258	0.0379
28	0.0051	0.0225	0.0357
30	0.0042	0.0195	0.0332
32	0.0035	0.0170	0.0306
34	0.0029	0.0147	0.0279
36	0.0024	0.0127	0.0253
38	0.0020	0.0110	0.0228
40	0.0017	0.0096	0.0204
42	0.0014	0.0083	0.0182
44	0.0012	0.0072	0.0162
46	0.0010	0.0062	0.0144
48	0.0009	0.0054	0.0127
50	0.0007	0.0047	0.0112
52	0.0006	0.0040	0.0099
54	0.0005	0.0035	0.0087
56	0.0005	0.0030	0.0076
58	0.0004	0.0026	0.0067
60	0.0003	0.0023	0.0059

Calculation of Volumes

In order to calculate regional volumes in the system, we must know the flow rates out of each region. Suppose we have this information; namely

$$q_{1,\text{out}} = 0$$
$$q_{2,\text{out}} = 0$$
$$q_{3,\text{out}} = 0.75 \text{ l/s}$$

Then, from Equation (16)

$$\begin{bmatrix} V_1 \\ V_2 \\ V_3 \end{bmatrix} = \begin{bmatrix} (0.3192 - 1) & 0.5630 & 0.0761 \\ 00.442 & (0.3896 - 1) & 0.5474 \\ 0.0000 & 0.0306 & (0.3511 - 1) \end{bmatrix}^{-1} \cdot \begin{bmatrix} 0 \\ 0 \\ (-0.75)\cdot(8) \end{bmatrix} = \begin{bmatrix} 8.79 \\ 9.32 \\ 9.69 \end{bmatrix}$$

These are the effective volumes monitored by the three probes. The total volume is calculated to be 27.8. The true volume of the system is 25; thus there is an 11% error in volume introduced by treating the twenty-five region system as three regions.

Calculated Residence Time Distribution

Only region 3 connects to the output; therefore the normalized response at 3 to an impulse at the input (region 1) gives the residence time distribution. This response is plotted in Figure 4 and compared with the true residence time distribution.

Steady State Responses

From the **P** matrix we can calculate the response in any region that would result from a steady tracer input into any other region. From Equation (29)

$$\mathbf{S} = \begin{bmatrix} (1 - 0.3192) & -0.5630 & -0.0761 \\ -0.0443 & (1 - 0.3896) & -0.5474 \\ 0.0000 & -0.0306 & (1 - 0.3511) \end{bmatrix}^{-1} = \begin{bmatrix} 1.58 & 1.78 & 1.69 \\ 0.12 & 1.85 & 1.57 \\ 0.01 & 0.09 & 1.62 \end{bmatrix}$$

For the **S** matrix, the concentration of the steady inlet flow into any region i is assumed to be

$$f_i = \frac{1}{p_{\text{in},1}} = \frac{V_i}{q_{\text{in},i}}$$

Thus, the tracer concentration in the cell immediately after the tracer is introduced will be unity. Since the tracer continues to enter the cell at the same rate, and there is (generally) incomplete washout and eventually tracer reentering from other cells, the final steady concentration in cell i will be greater than unity. This steady concentration in cell i has the numerical value s_{ii}. A region that does not connect to the inlet station can be considered as a limiting case where $q_{\text{in},i} \to 0$ and $f_i \to \infty$, so that at time 0^+ the concentration in the cell will be unity.

The s matrix shows that there is little backflow since all the elements below the main diagonal are quite small. For instance, a steady flow of (9.69) mmole of tracer/s into region III would cause a steady concentration of 1.61 mmole/l of tracer in region III and a steady tracer concentration of 0.09 mmole/l in region III.

Redundant Data with Errors

Suppose the tracer record for the three regions above contains small random errors. Suppose also that a long data record (more than four points in time) is available, so that there is some redundancy. Table 2 gives such a record. Random numbers with a mean of 0 and a standard deviation of 0.0003 have been added to the data of Table 1 to simulate noisy data. The readings are for regions 1, 2, and 3 (cells 11, 13, and 15 in the data generating model) at discrete times 0, Δt, $2\Delta t$, $3\Delta t$, $4\Delta t$, $5\Delta t$, and $6\Delta t$, where $\Delta t = 8$ s.

Using the noisy data for the first four values of time (no redundancy), we find from Equation (50)

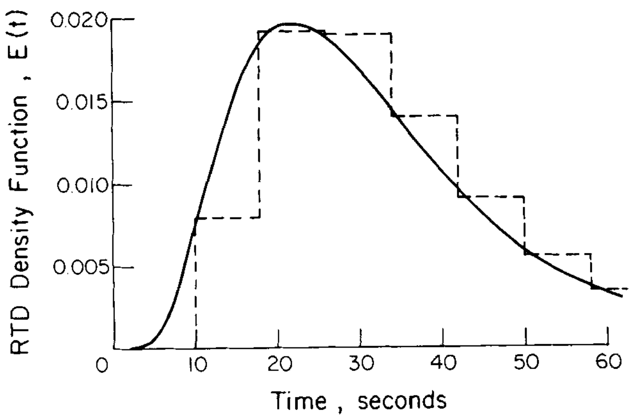

Fig. 4. Comparison of the true RTD and the discrete time compartmental model RTD.

$$\mathbf{P} = \begin{bmatrix} 0.2766 & 0.6135 & 0.1749 \\ 0.0755 & 0.2644 & 0.4615 \\ -0.0307 & 0.1130 & 0.4080 \end{bmatrix}$$

The coefficients differ by as much as a factor of 3 from those found for the noise free data.

We can improve on these estimates by making use of more data and using the least-square regression technique of Equation (55) with

$$\begin{matrix} \mathbf{C}(0) \\ \mathbf{C}(1) \\ \mathbf{C}(2) \\ \mathbf{C}(3) \\ \mathbf{C}(4) \\ \mathbf{C}(5) \end{matrix} = \begin{matrix} [00.372 & 0.0543 & 0.0160] \\ [0.0139 & 0.0427 & 0.0381] \\ [0.0059 & 0.0255 & 0.0377] \\ [0.0024 & 0.0152 & 0.0282] \\ [0.0008 & 0.0084 & 0.0182] \\ [0.0007 & 0.0044 & 0.0119] \end{matrix}$$

and

$$\begin{matrix} \mathbf{C}(1) \\ \mathbf{C}(2) \\ \mathbf{C}(3) \\ \mathbf{C}(4) \\ \mathbf{C}(5) \\ \mathbf{C}(6) \end{matrix} = \begin{matrix} [0.0139 & 0.0427 & 0.0381] \\ [0.0059 & 0.0255 & 0.0377] \\ [0.0024 & 0.0152 & 0.0282] \\ [0.0008 & 0.0084 & 0.0182] \\ [0.0007 & 0.0044 & 0.0119] \\ [0.0007 & 0.0029 & 0.0068] \end{matrix}$$

which gives

$$\mathbf{P} = \begin{bmatrix} 0.32 & 0.70 & 0.10 \\ 0.04 & 0.31 & 0.49 \\ 0.00 & 0.08 & 0.39 \end{bmatrix}$$

By comparison, the elements in this matrix differ by less than a factor of 1.5 from the p_{ij} found for noise free data. Thus, a substantial improvement is obtained by the least-square technique. The second and third columns sum to approximately 1.0, while the first column sums to only 0.36, indicating (correctly) a flow into region I from the inlet station. The volumes calculated from Equation (16) are

$$\begin{bmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \\ \mathbf{V}_3 \end{bmatrix} = \begin{bmatrix} (0.32-1) & 0.70 & 0.10 \\ 0.04 & (0.31-1) & 0.49 \\ 0.0 & 0.08 & (0.39-1) \end{bmatrix}^{-1} \cdot \begin{bmatrix} 0 \\ 0 \\ -(0.75)\cdot(8) \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \\ \mathbf{V}_3 \end{bmatrix} = \begin{bmatrix} 10.21 \\ 8.35 \\ 10.93 \end{bmatrix}$$

which agrees quite well with the volumes calculated for noise free data. As before, the calculated volume is larger than the true volume of the system.

If a smaller Δt is used, then the fraction of fluid remaining in each region after a transition is larger; for instance, if Δt is chosen as 2 rather than $\Delta t = 8$, the **P** matrix becomes

Table 2. Tracer Data for Cells 11, 13, and 15 of the Simulated Flow System of Figure 3 with Added Noise ($\mu = 0, \sigma = 0.003$)

Time	Cell 1	Cell 13	Cell 15
0	0.2002	−0.0006	0.0001
2	0.1313	0.0069	0.0001
4	0.0915	0.0268	0.0004
6	0.0659	0.0426	0.0032
8	0.0487	0.0513	0.0083
10	0.0372	0.0543	0.0160
12	0.0291	0.0545	0.0234
14	0.0229	0.0510	0.0295
16	0.0175	0.0470	0.0350
18	0.0139	0.0427	0.0381
20	0.0120	0.0379	0.0401
22	0.0091	0.0336	0.0397
24	0.0079	0.0293	0.0392
26	0.0059	0.0255	0.0377
28	0.0058	0.0224	0.0356
30	0.0042	0.0196	0.0332
32	0.0039	0.0170	0.0304
34	0.0024	0.0152	0.0282
36	0.0023	5.0131	0.0254
38	0.0019	0.0111	0.0222
40	0.0016	0.0103	0.0205
42	0.0008	0.0084	0.0182
44	0.0011	0.0073	0.0155
46	0.0012	0.0061	0.0146
48	0.0005	0.0053	0.0127
50	0.0007	0.0044	0.0119
52	0.0008	0.0038	0.0099
54	0.0007	0.0035	0.0090
56	0.0007	0.0031	0.0076
58	0.0007	0.0029	0.0068
60	0.0009	0.0024	0.0058

$$\mathbf{P} = \begin{bmatrix} 0.73 & 0.29 & -0.10 \\ 0.03 & 0.79 & 0.27 \\ 0.00 & 0.01 & 0.77 \end{bmatrix}$$

For this case we find

$$\begin{bmatrix} \mathbf{V}_1 \\ \mathbf{V}_2 \\ \mathbf{V}_3 \end{bmatrix} = \begin{bmatrix} 8.31 \\ 10.14 \\ 6.96 \end{bmatrix}$$

Here the total volume is 25.41 which is much closer to the true volume.

NOTATION

$c_i(m)$ = concentration in the i^{th} region at time $m\Delta t$
$c_i(t)$ = concentration in the i^{th} region at time t
$\mathbf{C}(m)$ = concentration row vector at time $m\Delta t$
$\mathbf{C}(t)$ = concentration row vector at time t
$\overline{\mathbf{C}}(m)$ = augmented concentration row vector with an accumulating station (at time $m\Delta t$)
$E(t)$ = residence time distribution
$f_i(m)$ = concentration of stream from the inlet station to region i (at time $m\Delta t$)
$\mathbf{F}(m)$ = input concentration row vector at time $xn\Delta t$
$\mathbf{I}$ = identity matrix
m = integer multiplying Δt
n = number of regions
p_{ij} = fractional input coefficient from region i to region j
$\mathbf{P}$ = matrix of fractional input coefficients
$\mathbf{P}_{in}$ = matrix of fractional input coefficients from the in-

let station

$\bar{p}$ = fractional input matrix augmented to include an accumulating station

g_{ij} = volumetric flow rate from region i to region j

g'_{ij} = volumetric flow rate from region i to region j for stirred-tank network model

r_{ij} = fractional input coefficient from tank i to tank j for stirred-tank network, see Equation (34) for special definition of r_{jj}

R = matrix of fractional input coefficients for the stirred-tank network model

$\mathbf{R}_{in}$ = matrix of fractional input coefficients from the inlet station top the stirred-tank network model

s_{ij} = steady response at region j to a steady tracer input into region i

S = matrix of steady response coefficients

t = time

V_i = volume of the i^{th} region

V_i' = volume of the i^{th} tank in the stirred-tank network model

V = volume column vector

V' = volume column vector for the stirred tank network model

α_i = coefficients in the Caley-Hamilton equation

λ = eigenvalue

Δt = single transition time interval

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The Permeation of Gases Through Hollow Silicone Rubber Fibers: Effect of Fiber Elasticity on Gas Permeability

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The permeation of oxygen, nitrogen, argon, and synthetic air through hollow silicon rubber fibers was studied between 0° and 40°C and at gauge pressures of up to 3.45×10^5 N/m² (50 lb/in.² abs). The study was conducted in a permeator module in which the hollow fibers were pressurized externally. Strain measurements with single fibers showed this mode of operation to be preferable to internal pressurization. The gas permeation rates were markedly affected by dimensional changes of the hollow fibers under external pressure. These changes were predicted satisfactorily by a modification of Varga's (1966) deformation analysis of thick-walled elastic tubes. The extent of air separation achieved in the permeator was in agreement with that calculated from theoretical models. It is conjectured that the performance of such a permeator may be improved in certain cases if the fibers are under suitable initial tension.

SCOPE

The development of hollow fiber permeators has been one of the most important advances in membrane separation technology in recent years. Such permeators, which use hollow polymer fibers as separation barriers, offer important advantages over permeator modules employing spiral or flat sheet membranes. One advantage is that a much larger membrane area can be packed per unit permeator volume, thus greatly reducing capital investment costs. Another advantage is that hollow fiber permeators do not require costly membrane supports and are more damage-resistant than other types of permeators. Hollow fiber permeators are being used on a large scale for water desalination and purification and are also being considered for the separation of various gas mixtures.

Silicone rubber is a membrane material of particular interest for gas separations because it exhibits a very high gas permeability compared to other polymers. For example, silicone rubber membranes, either in hollow fiber or sheet form, have been employed for biomedical applications and are potentially useful for the inerting of fuel tanks of jet transports and in the nuclear industry.

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