MODELING AND SIMULATION OF DEEP BED FILTRATION: A Stochastic Compartmental Model

by

SONG-TIEN CHOU

B. S., National Taiwan University, 1974

M. S., Kansas State University, 1982

A MASTER'S REPORT

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Statistics

KANSAS STATE UNIVERSITY

Manhattan, Kansas

1984

Approved by:

R Nassar

Major Professor

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   II: m_{12}=1.0/h, m_{13}=2.0/h, m_{21}=0.0/h, m_{24}=1.0/h,
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I. INTRODUCTION

Deep-bed filters are of importance in purification of potable water and in treatment of wastewater. The solid-liquid separation in deep-bed filters has been modeled deterministically by various investigators using the phenomenological equation of kinetics (Iwasaki, 1937; Ives, 1960, 1961; Camp, 1964) and the trajectory analysis (O'Melia and Stumm, 1967; Yao et al., 1971; Payatakes, 1973; Rajagopalan and Tien, 1976, 1979; Tien et al., 1978 a,b).

Deep bed filtration involves flow of mesoscopic particles through randomly distributed passages; thus, it tends to be stochastic in nature. Stochastic models of the Markovian type, therefore, have also been used to model the deep bed filtration (Litwiniszyn, 1963, 1966, 1967, 1968 a,b, 1969; Hsu, 1981; Hsu and Fan, 1984; Fan et al., 1984). Stochastic process models are often relatively simple and easy to apply, thereby providing a viable alternative to deterministic models. In Litwiniszyn's pure birth model (1963), the entire bed is considered as one state, and the number of blocked pores is taken as a random variable. In his birth-death process model (1966), the number of trapped particles over the entire bed is a random variable. These works of Litwiniszyn have not received sufficient recognition since the parameters of resultant models are not explicitly related to measurable variables of the process (e.g., pressure drop and concentration). Hsu (1981), Hsu and Fan (1984), and Fan et al. (1984) have extended the pure birth and birth-death process models by incorporating them with the Carman-Kozeny equation to simulate the pressure drop dynamics of a deep-bed filter under constant flow conditions. However, the concentration of the filtrate as a function of time is also of vital importance in filtration. Thus, it is highly desirable that a model be developed for predicting the concentration of suspended particles both in the filter and in the effluent.

In this work, a deep-bed filter is considered to be an open flow system composed of an arbitrary number of sections or compartments distributed in the axial direction; a stochastic compartment model is employed to describe the concentration dynamics of suspended particles in those sections of the bed and at the exit. For illustration, six sets of parameters are used to simulate the concentration dynamics of suspended particles in the filtrates of a two compartment filter. Finally, the applicability of this model is demonstrated by analyzing Eliassen's experimental data.

II. MATHEMATICAL MODEL

1. Compartmental Model

Consider that a deep-bed filter is divided into n compartments distributed in the axial direction or the direction of flow, as shown in Figure 1; each compartment consists of one liquid phase, occupied by the liquid, and one solid phase, occupied by the grain medium. Let L_i denote the liquid phase and D_i the solid phase in compartment i. We assume that the particles in suspension enter the system through the liquid phase of the first compartment and exit from the system through the liquid phase of the last compartment. Without loss of generality, we assume that suspension enter the system at a constant volumetric rate of q and a constant particle concentration of C_0. The rate of particles entering the system through the feed stream, X, may be obtained as

$$X = qC_0 \tag{1}$$

In a small time interval $(t, t+\Delta t)$, a particle in the liquid phase, L_i, may (1) remain in L_i, (2) move to the liquid phase in another compartment, L_j, (3) move to the solid phase, or (4) exit from the system. A particle in the solid phase, D_i, may (1) remain in D_i, or (2) move to the liquid phase. This process is depicted in Figure 1. This system defines a Markov process with 2n states (S_i, i = 1, 2, ..., 2n). For convenience, we let the first n states (S_i, i = 1, 2, ..., n) belong to the liquid phase (hence, called liquid states hereafter), and the second n states (S_i, i = n+1, n+2, ..., 2n) belong to the solid phase (hence, called solid states hereafter), respectively (see Figure 1).

Let $m_{ij}(t)$, i, j = 1, 2, ..., 2n, be the intensity functions of the Markov process (see, e.g., Chiang, 1980). From the definitions,

$$m_{ij}(t)\Delta t + o(\Delta t)$$

$$= \Pr[\text{a particle in state } i \text{ at time } t \text{ will move to state } j \text{ at time } t+\Delta t,\ j \neq i], \qquad (2)$$

$$\mu_i(t)\Delta t + o(\Delta t)$$

$$= \Pr[\text{a particle in state } i \text{ at time } t \text{ will exit at time } t+\Delta t], \qquad (3)$$

$$1 - [\sum_{\substack{j=1\\ j\neq i}}^{2n} m_{ij}(t)\Delta t + \mu_i(t)\Delta t] + o(\Delta t)$$

$$= \Pr[\text{a particle in state } i \text{ at time } t \text{ will remain in the same state at time } t+\Delta t]$$

$$= 1 + m_{ii}(t)\Delta t + o(\Delta t) \qquad (4)$$

and

$$p_{ij}(t,\ t+\Delta t)$$

= transition probability that a particle in state i at time t will be in state j at time $t+\Delta t$, $i,j = 1, 2, \ldots, 2n$.

where $o(\Delta t)$ satisfies the condition that

$$\lim_{\Delta t \to 0} \frac{o(\Delta t)}{\Delta t} = 0,$$

From Eq. 4, we have

$$m_{ii}(t) = -[\sum_{\substack{j=1\\ j\neq i}}^{2n} m_{ij}(t) + \mu_i(t)],\quad i = 1, 2, \ldots, 2n \qquad (5)$$

Let $\underline{P}(\tau,t)$ be the matrix of transition probabilities $[p_{ij},(\tau,t)]$. It can be shown (Chiang, 1980) that $\underline{P}(\tau,t)$ satisfies the Kolmogorov forward differential equation, i.e.,

$$\frac{d}{dt}\underline{P}(\tau,t) = \underline{P}(\tau,t)\underline{M}(t) \tag{6a}$$

with the initial condition

$$\underline{P}(\tau,\tau) = \underline{I} = \text{identity matrix} \tag{6b}$$

where $\underline{M}(t)$ is the matrix of intensity functions, $m_{ij}(t)$.

For a time homogeneous process (i.e., intensity functions are not dependent on time), Eq. 6 becomes

$$\frac{d}{dt}\underline{P}(t-\tau) = \underline{P}(t-\tau)\underline{M} \tag{7a}$$

with the initial condition

$$\underline{P}(0) = \underline{I} = \text{identity matrix} \tag{7b}$$

The solutions of Eqs. 6 and 7 depend on the intensity matrix $\underline{M}$.

For deep bed filtration, it is reasonable to assume that, in a very small time interval $(t, t+\Delta t)$,

1. the transition probability that a particle moves from the solid phase of compartment i to that of compartment j is $o(\Delta t)$, i.e.,

$$P_{ij}(t, t+\Delta t) = o(\Delta t)$$

or (8a)

$$m_{ij}(t) = 0,$$

$$i,j = n+1, n+2, \ldots, 2n, \quad i \neq j$$

2. the transition probability that a particle moves from the liquid phase to the solid phase, or from the solid phase to the liquid phase, where both phases are not in the same compartment, is $o(\Delta t)$, i.e.,

$$p_{ij}(t,\ t+\Delta t) = o(\Delta t)$$

or (8b)

$$m_{ij}(t) = 0\ ,$$

$$|i - j| > n\ ,$$

3. the transition probability that a particle moves more than one compartment is $o(\Delta t)$, i.e.,

$$p_{ij}(t,\ t+\Delta t) = o(\Delta t)$$

or (8c)

$$m_{ij}(t) = 0$$

$$|i - j| > 1$$

$$i,j = 1,\ 2,\ \ldots,\ n$$

Since particles exit from the filter only through the liquid phase of the last compartment, we have

$$\mu_i = 0 \quad \text{for} \quad i \neq n \tag{8d}$$

Based on these assumptions, we have(see Figure 2).

$$
\underline{M}(t) = \begin{array}{c} L \\ \\ D \end{array}
\left[\begin{array}{cccccc:cccccc}
\multicolumn{6}{c}{L} & \multicolumn{6}{c}{D} \\
m_{11}(t) & m_{12}(t) & 0 & \cdots & 0 & 0 & m_{1,n+1}(t) & 0 & 0 & \cdots & 0 & 0 \\
m_{21}(t) & m_{22}(t) & m_{23}(t) & \cdots & 0 & 0 & 0 & m_{2,n+2}(t) & 0 & \cdots & 0 & 0 \\
0 & m_{32}(t) & m_{33}(t) & \cdots & 0 & 0 & 0 & 0 & m_{3,n+3}(t) & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & m_{n-1,n-1}(t) & m_{n-1,n}(t) & 0 & 0 & 0 & \cdots & m_{n-1,2n-1}(t) & 0 \\
0 & 0 & 0 & \cdots & m_{n,n-1}(t) & m_{n,n}(t) & 0 & 0 & 0 & \cdots & 0 & m_{n,2n}(t) \\
\hdashline
m_{n+1,1}(t) & 0 & 0 & \cdots & 0 & 0 & m_{n+1,n+1}(t) & 0 & 0 & \cdots & 0 & 0 \\
0 & m_{n+2,2}(t) & 0 & \cdots & 0 & 0 & 0 & m_{n+2,n+2}(t) & 0 & \cdots & 0 & 0 \\
0 & 0 & m_{n+3,3}(t) & \cdots & 0 & 0 & 0 & 0 & m_{n+3,n+3}(t) & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & m_{2n-1,n-1}(t) & 0 & 0 & 0 & 0 & \cdots & m_{2n-1,2n-1}(t) & 0 \\
0 & 0 & 0 & \cdots & 0 & m_{2n,n}(t) & 0 & 0 & 0 & \cdots & 0 & m_{2n,2n}(t)
\end{array}\right] \qquad (9)
$$

For the case where the intensity functions or elements of the matrix $\underline{M}(t)$ are constant, the solution of the first-order differential equation, Eq. 7, is given as (see e.g., Chiang, 1980)

$$\underline{P}(t-\tau) = \underline{Q}(r)\underline{E}(t-\tau)\underline{Q}^{-1}(r) \tag{10}$$

where

$$\underline{Q}(r) = \begin{bmatrix} B_{r,1}(\rho_1) & B_{r,1}(\rho_2) & \cdots & B_{r,1}(\rho_{2n}) \\ B_{r,2}(\rho_1) & B_{r,2}(\rho_2) & \cdots & B_{r,2}(\rho_{2n}) \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ B_{r,2n}(\rho_1) & B_{r,2n}(\rho_2) & \cdots & B_{r,2n}(\rho_{2n}) \end{bmatrix} \tag{11a}$$

and

$$\underline{E}(t-\tau) = \begin{bmatrix} e^{\rho_1(t-\tau)} & 0 & 0 & \cdots & 0 \\ 0 & e^{\rho_2(t-\tau)} & 0 & \cdots & 0 \\ 0 & 0 & e^{\rho_3(t-\tau)} & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & e^{\rho_{2n}(t-\tau)} \end{bmatrix} \tag{11b}$$

Column k (k = 1, 2, ..., 2n) in $\underline{Q}(r)$ represents an eigenvector corresponding to the eigenvalue ρ_k. This is obtained as the r-th column of the adjoint matrix (transpose matrix of the cofactor) of the matrix $[\rho_k \underline{I} - \underline{M}]$.

Expanding Eq. 10 yields

$$p_{ij}(t-\tau) = \sum_{k=1}^{2n} B_{ri}(\rho_k) \frac{Q_{jk}(r)}{|\underline{Q}(r)|} \exp[\rho_k(t - \tau)] \tag{12}$$

where $Q_{jk}(r)$ is the cofactor of the element $B_{rj}(\rho_k)$ of the matrix $\underline{Q}(r)$, $|\underline{Q}(r)|$ is the determinant of $\underline{Q}(r)$, and ρ_k's are the eigenvalues of the intensity matrix $\underline{M}$ and are assumed to be real and distinct. A solution is also known for the case of nondistinct or overlapping eigenvalues (see, e.g., Chiang, 1980). If the entire bed is considered simply as one compartment, Eq. 7 can be solved analytically; the resultant solution is given in APPENDIX A.

If the intensity functions, $m_{ij}(t)$, are not constant and are continuous functions of time, Eq. 7 can be solved uniquely; however, the resultant solution may not be in closed form (Bellman, 1960). It may be expressed as

$$\underline{P}(\tau,t) = \underline{G}(\tau,t) = \underline{I} + \int_{\tau}^{t} \underline{G}(\tau,\xi)\underline{M}(\xi)\, d\xi \tag{13}$$

The matrix $\underline{G}(\tau,t)$ may be obtained iteratively according to the following matrix sequence (see, e.g., Bellman, 1960).

$$\underline{G}_0 = \underline{I} = \text{identity matrix}$$

$$\underline{G}_{m+1} = \underline{I} + \int_{\tau}^{t} \underline{G}_m\, \underline{M}(\xi)\, d\xi \tag{14}$$

It can be shown that Eq. 14 reduces to the time homogeneous solution if $\underline{M}$ is constant.

2. Internal Particle Distribution

To gain insight into the performance of a deep-bed filter, it is essential that the spatial distribution of suspended particles in the bed should be determined as a function of time. In other words, it should be of interest to determine the distribution of particles in suspension (liquid phase) or on the solid medium (solid phase) over the different compartments of the bed. It is assumed that the process is time homogeneous (i.e., the intensity functions are not functions of time) and N_0 particles enter instantaneously the system only through the liquid phase of the first compartment at time τ. It is also assumed that these particles have the same characteristics (e.g., the same shape and size) and behave independently of one another. Then, each of the N_0 particles originally in state 1 will be in one of the 2n states with probability $p_{1j}(t-\tau)$, $j = 1,2,\ldots,2n$, which is obtained from Eq. 10 with $\underline{M}$ specified by Eq. 9, or be outside the system (i.e., in the surroundings) with probability $r_{1s}(t-\tau)$, which may be obtained from the following equation;

$$r_{1s}(t-\tau) = \int_{\tau}^{t} p_{1n}(t-\xi)\,\mu_n\,d\xi \tag{15}$$

Hence, if N_0 particles are initially in state 1, then the number of suspended particles in each of the 2n states at time t follows a multinominal distribution (see, e.g., Rohatgi, 1976). Let $Y_i(t)$, $i = 1,2,\ldots,2n$, be the random variable representing the number of suspended particles in state i at time t. Then, the joint density of $(Y_1(t), Y_2(t), \ldots, Y_n(t))$ is

$$\Pr[Y_1(t)=y_1(t),\ Y_2(t)=y_2(t),\ \ldots,\ Y_n(t)=y_n(t)]$$

$$= \frac{(N_0)!}{\{\prod_{i=1}^{n} y_i(t)!\}\{N_0-\sum_{i=1}^{n} y_i(t)\}!}\left\{\prod_{i=1}^{n}[p_{1i}(t-\tau)]^{y_i(t)}\right\}\left\{1-\sum_{i=1}^{n} p_{1i}(t-\tau)\right\}^{[N_0-\sum_{i=1}^{n} y_i(t)]} \tag{16}$$

The distribution of the numbers of suspended particles over the states k ($k = n+1, n+2, \ldots, 2n$) in the solid phase may also be obtained from the multinominal distribution as

$$\Pr[Y_{n+1}(t)=y_{n+1}(t),\ Y_{n+2}(t)=y_{n+2}(t),\ \ldots,\ Y_{2n}(t)=y_{2n}(t)]$$

$$= \frac{(N_0)!}{\{\prod_{k=n+1}^{2n} y_k(t)!\}\{N_0 - \sum_{k=n+1}^{2n} y_k(t)\}!} \{\prod_{k=n+1}^{2n} [p_{1k}(t-\tau)]^{y_k(t)}\}\{1 - \sum_{i=1}^{n} p_{1k}(t-\tau)\}^{[N_0 - \sum_{k=n+1}^{2n} y_k(t)]} \tag{17}$$

Then, the mean and variance of the number of suspended particles in any state i ($i = 1,2,\ldots,2n$) at time t are

$$E[Y_i(t)] = N_0\, p_{1i}(t-\tau) \tag{18}$$

$$\mathrm{Var}[Y_i(t)] = N_0\, p_{1i}(t-\tau)[1 - p_{1i}(t-\tau)] \tag{19}$$

If the particles enter the filter at a constant rate of X during the time interval (τ, t), then $Xd\xi$ particles will enter the bed during the time interval $(\xi, \xi+d\xi)$ where $\tau<\xi<t$. The mean and variance of the number of these particles in any state $i(i=1,2,\ldots,2n)$ at time t are, respectively,

$$E[dY_i(t)] = Xd\xi\, p_{1i}(t-\xi) \tag{20a}$$

$$\mathrm{Var}[dY_i(t)] = Xd\xi\, p_{1i}(t-\xi)[1 - p_{1i}(t-\xi)] \tag{20b}$$

Integration of Eqs. 20a and 20b over (τ, t), subject to the initial condition,

$$Y_i(0) = 0, \qquad i = 1, 2, \ldots, 2n$$

$$E[Y_i(t)] = X \int_{\tau}^{t} p_{1i}(t-\xi)d\xi \tag{21a}$$

$$Var[Y_i(t)] = X \int_{\tau}^{t} p_{1i}(t-\xi)[1 - p_{1i}(t-\xi)]d\xi \tag{21b}$$

Furthermore, if a particle is trapped permanently on the grain medium (i.e., the states in the solid phase are absorbing), the distribution of the numbers of suspended particles over all the states in the solid phase at time t provided that N_0 particles entered the bed at time τ, is also multinominal as given in Eq. 16, except that $p_{1k}(t-\tau)$ are replaced by $r_{1k}(t-\tau)$, which are obtained from the following equation;

$$r_{1k}(t-\tau) = \int_{\tau}^{t} p_{1,k-n}(t-\xi)m_{k-n,k}\, d\xi, \quad k = n+1,n+2,\ldots,2n \tag{22}$$

$p_{1,k-n}(t-s)$ in this expression is obtained from Eq. 7 with $\underline{M}$ being an n x n matrix specified as follows

$$\underline{M} = \begin{bmatrix} m_{11} & m_{12} & 0 & \cdots & 0 & 0 \\ m_{21} & m_{22} & m_{23} & \cdots & 0 & 0 \\ 0 & m_{32} & m_{33} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & m_{n-1,n-1} & m_{n-1,n} \\ 0 & 0 & 0 & \cdots & m_{n,n-1} & m_{nn} \end{bmatrix} \tag{23}$$

where

$$m_{ii} = -(m_{i,i-1} + m_{i,i+1} + m_{i,n+i}), \text{ for } i = 1,2,\ldots,n-1$$

$$m_{nn} = -(m_{n,n-1} + m_{n,2n} + \mu_n)$$

$$\Pr[Y_{n+1}(t)=y_{n+1}(t),\ Y_{n+2}(t)=y_{n+2}(t),\ \ldots,\ Y_{2n}(t)=y_{2n}(t)]$$

$$= \frac{(N_0)!}{\{\prod_{k=n+1}^{2n} y_k(t)!\}\{N_0 - \sum_{k=n+1}^{2n} y_k(t)\}!} \{\prod_{k=n+1}^{2n} [r_{1k}(t-\tau)]^{y_k(t)}\}$$

$$\{1 - \sum_{k=n+1}^{2n} r_{1k}(t-\tau)\}^{[N_0 - \sum_{k=n+1}^{2n} y_k(t)]} \tag{24}$$

and the mean and variance of the number of suspended particles in the solid phase of each compartment at time t are, respectively,

$$E[Y_k(t)] = N_0\ r_{1k}(t-\tau) \tag{25a}$$

$$\mathrm{Var}[Y_k(t)] = N_0\ r_{1k}(t-\tau)[1 - r_{1k}(t-\tau)]\ , \tag{25b}$$

$$k = n+1,\ n+2,\ \ldots,\ 2n.$$

These results are obtained under the condition that N_0 suspended particles are fed instantaneously into the liquid phase of the first compartment at time τ. If the suspended particles enter the filter at a constant rate of X over the time interval $(\tau,\ t)$, the mean and variance of the number of suspended particles in the solid phase of each compartment at time t are, respectively,

$$E[Y_k(t)] = X \int_{\tau}^{t} r_{1k}(t-\xi)\ d\xi \tag{26a}$$

$$\mathrm{Var}[Y_k(t)] = X \int_{\tau}^{t} r_{1k}(t-\xi)[1 - r_{1k}(t-\xi)]\ d\xi \tag{26b}$$

3. Distribution of Particles in the Effluent

Suppose that N_0 particles are initially fed instantaneously into the liquid phase of the first compartment; at time t, each of these particles will exit from the system with probability $r_{1s}(t-\tau)$, which is obtained from Eq. 15, or remain in the bed with probability $[1 - r_{1s}(t-\tau)]$. Hence the number of suspended particles in the surroundings (i.e. outside the bed) at time t has a binominal distribution. Let $Y_s(t)$ be the random variable representing the number of suspended particles in the effluent at time t, then we have

$$Pr[Y_s(t) = y_s(t)]$$

$$= \frac{N_0!}{y_s(t)!\,[N_0 - y_s(t)]!}\,[r_{1s}(t-\tau)]^{y_s(t)}\,[1 - r_{1s}(t-\tau)]^{[N_0 - y_s(t)]} \qquad (27)$$

The mean and variance of the number of suspended particles in the surroundings at time t are expressed, respectively, as

$$E[Y_s(t)] = N_0\, r_{1s}(t-\tau) \qquad (28)$$

$$Var[Y_s(t)] = N_0\, r_{1s}(t-\tau)[1 - r_{1s}(t-\tau)] \qquad (29)$$

If the suspended particles enter the filter at a constant rate of X over the time interval (τ, t), the mean and variance of the number of suspended particles in the effluent at time t are, respectively,

$$E[Y_s(t)] = X \int_\tau^t r_{1s}(t-\xi)\, d\xi \qquad (30)$$

$$Var[Y_s(t)] = X \int_\tau^t r_{1s}(t-\xi)[1 - r_{1s}(t-\xi)]\, d\xi \qquad (31)$$

III. NUMERICAL SIMULATION AND PARAMETER ESTIMATION

In the previous sections we have formulated expressions for the expected numbers of suspended particles in the liquid and solid phases in each compartment of the bed as functions of time. For experimental purposes, the expected number concentration can be recovered by dividing the expected numbers of particles by the respective volume. For instance, let $C_i(t)$ be the particle concentration of the filtrate sampled from the end of compartment i, i=1,2,...n, during the time interval $(t, t+\Delta t)$. Then, the mean of $C_i(t)$, $E[C_i(t)]$, for a deep-bed filter with a constant volumetric flow rate of q and a constant suspension concentration of $C_0 (C_0 = X/q)$ is

$$E[C_i(t)] = \frac{E[Y_i(t)(\delta q/q)\ m_{i,i+1}\Delta t]}{(\delta q \Delta t)} = \frac{E[Y_i(t) m_{i,i+1}\Delta t]}{q\Delta t}\ , \qquad (32)$$

$$i = 1, 2, \ldots, n-1$$

where δq is rate of sampling from each compartment. Substitution of Eq. 21a into Eq. 32 and rearrangement of the resultant expression yield

$$E[C_i(t)] = (X/q) \int_{\tau}^{t} p_{1i}(t-\xi) m_{i,i+1} d\xi$$

$$= (C_0) \int_{\tau}^{t} p_{1i}(t-\xi) m_{i,i+1} d\xi$$

or

$$E[C_i(t)/C_0] = \int_{\tau}^{t} p_{1i}(t-\zeta) m_{i,i+1} d\xi \qquad i = 1, 2, \ldots, n-1 \qquad (33)$$

For i = n, i.e., the last compartment, we have

$$E[C_n(t)/C_0] = \int_{\xi}^{t} p_{1n}(t-\zeta) u_n d\zeta \qquad (34)$$

Similarly, the variance of $C_i(t)$, $Var[C_i(t)]$, is obtained as

$$\mathrm{Var}[C_i(t)/C_0] = (m^2_{i,i+1}/X) \int_\tau^t p_{1i}(t-\xi)[1 - p_{1i}(t-\xi)]d\xi \qquad (35)$$

$$i = 1, 2, \ldots, n-1.$$

For i = n, we have

$$\mathrm{Var}[C_n(t)/C_0] = (u^2_n/X) \int_\tau^t p_{1n}(t-\xi)[1 - p_{1n}(t-\xi)]d\xi \qquad (36)$$

1. Numerical Simulation

In the derivation of the present model, it is assumed that the particles in the suspension are uniform and spherical, Thus, the ratio of $C_i(t)$ to the initial particle concentration of the suspension, C_0, is essentially equal to that of the weight concentration, $W_i(t)$, to the initial weight concentration of the suspension, W_0. If the intensity functions of this system are known a priori, we can simulate the concentration dynamics of the filtrate sampled from each compartment of the bed through the following procedure:

1. Obtain the transition probabilities, $p_{1j}(t-\tau)$, by solving numerically the system of differential equations, Eq. 7, by means of a finite difference scheme or the Monte Carlo method.
2. Calculate $E[C_i(t)/C_0]$ from Eq. 33 or $E[C_n(t)/C_0]$ from Eq. 34.

For illustration, six sets of parameters have been used in simulating the case where the bed is divided into 2 compartments. The results are shown in Figures 3 through 5. In Figure 3, lines I-1 and I-2 represent, respectively, the concentration dynamics of the filtrates from compartments

1 and 2 for the case where the intensity function, m_{21}, is equal to zero (i.e., the backmixing between compartments is insignificant), while lines II-1 and II-2 are for the case where the backmixing between compartments is significant. Figure 4 compares the concentration dynamics of the filtrates for different values of m_{12} and μ_2 with other intensity functions fixed. Finally, Figure 5 shows the case where the solid parts are absorbing, i.e., once the suspended particles are trapped by the solid medium, they will not return to the liquid phase.

2. Parameter Estimation

The parameters of the model can be estimated from the transition probabilities, $p_{1j}(t-\tau)$, which are related to the weight concentrations of the filtrates sampled from the liquid phase of each compartment as shown in Eqs. 33 and 34. Values of parameters in the model are selected in such a way that they minimize the deviations between the observed (obs) and expected (exp) weight concentrations of the filtrates. The objective function used to measure the extent of deviation in this study is the sum of least square errors, i.e.,

$$O.F. = \sum_{i=1}^{n} (A_{obs} - A_{exp})_i^2 \qquad (37)$$

where

$$A = W_i(t)/W_0$$

A_{obs} is evaluated from an experimental data point, and A_{exp} from Eq. 33 or 34; the summation is over all data points. Among various minimization techniques available, a random search technique (Brooks, 1958; Fan et al., 1975; Chen and Fan, 1976) has been employed in this work since it is difficult to obtain the derivatives of the transition probability functions with respect to their parameters and the random search technique utilizes no derivatives in its algorithm (see APPENDIX B).

IV. DISCUSSION AND CONCLUSION

The present stochastic model is more general than the pure birth process and birth-death processes considered by earlier investigators (Litwiniszyn, 1963, 1966,; Hsu, 1982; Hus and Fan, 1984; and Fan et al., 1984) in that it is capable of modeling the dynamics of spatial distributions of suspended particles in the bed, and its parameters can be related to the measurable variable of the model, namely, concentration. Once the parameters, m_{ij} and u_n, are obtained, the distribution, mean and variance of the number of particles (and hence, the concentration of particles) in the liquid and solid phases inside the filter at any time t may be obtained from Eqs. 16, 20, and 21. Also, the distribution, mean and variance of the number of suspension particles in the effluent at time t may be obtained from Eqs. 27, 30, and 31.

To demonstrate its applicability, the experimental results of Eliassen (1935) have been analyzed in the light of the present model; the results are shown in Figure 6. In his experiments a down-flow filter, i.e., the direction of flow was downward through the bed, with the depth of 60 cm, was used to remove Fuller's earth suspended particles from water. The weight concentrations of the filtrates from different bed heights (4.27 cm, 11.89 cm, 27.13 cm, 42.37 cm, and 60 cm) were measured at different times (2 hrs, 12 hrs, 24 hrs, 36 hrs, 48 hrs, 58 hrs, 72 hrs, 83 hrs, and 96 hrs).

In the present work, Eliassen's filter is divided into 2 axial compartments (0 ~ 27.13 cm of the bed as the first compartment, 27.13 ~ 60 cm as the second compartment) in the direction of flow for convenience. Since the direction of flow in the Eliassen's bed is downward, it is reasonable to assume that the transition probability of a particle moving from compartment i to i-1 during a small time interval $(t, t+\Delta t)$ is $o(\Delta t)$, i.e., $m_{i,i-1} = 0$, or the upward migration of particle is negligible. The intensity matrix, $\underline{M}$, is expresses as

$$\underline{M} = \begin{bmatrix} -(m_{12} + m_{13}) & m_{12} & m_{13} & 0 \\ 0 & -(m_{24} + \mu_2) & 0 & m_{24} \\ m_{31} & 0 & -m_{31} & 0 \\ 0 & m_{42} & 0 & -m_{42} \end{bmatrix} \qquad (38)$$

Computational subroutines are available for determining the eigenvalues, ρ's, the matrix of eigenvectors, $\underline{Q}$, of the intensity matrix $\underline{M}$, and the inverse of a matrix (see, e.g., EIGRF and LEQ2C in the IMSL Library). We can obtain the probability functions, $p_{1j}(t-\tau)$, from Eq. 10. To obtain the optimal set of parameters for the present model, we resorted to the random search technique (also see APPENDIX B), and used the sum of least square errors as the objective function. To reduce the computation time and the search effort, these parameters were estimated in a sequential manner, i.e., we applied the one-compartment model to estimate the first three parameters (m_{12}, m_{13}, and m_{31}) which are associated with compartment 1. Then, with these three parameters in hand, we applied the two-compartment model to estmate the second three parameters (m_{24}, m_{42}, and μ_2) which are associated with compartment 2. Finally, the six estimated parameters were used as the starting point to search for the optimal set of parameters. The parameters obtained are shown in Table 1. Comparison between the simulated results and experimental data are shown in Figure 6. Note that the agreement between experimental observations and the present model is sufficiently good, indicating that the present model is suitable for predicting the concentration dynamics of the filtrate in a deep bed filtration process.

The intensity functions, m_{ij} and μ_n, are functions of many factors, among which are the size distributions of collector grains and suspended particles, properties of the liquid and involved surfaces, filtration rate, bed porosity and suspension concentration. These intensity functions may be estimated through tracer experiments or, as for the Eliassen's example, from the observed concentrations of suspended particles in different sections of the bed. Estimation techniques as well as the correlation of the intensity functions with the characteristics of the bed and suspension, and operating conditions will be investigated in our futur work.

Table 1: Parameters of the Model Used for Describing Eliassen's Experimental Data

$m_{12} = 29.677\ h^{-1}$,	$m_{13} = 436.600\ h^{-1}$,	$m_{31} = 0.1385\ h^{-1}$
$\mu_2 = 16.713\ h^{-1}$,	$m_{24} = 18.432\ h^{-1}$,	$m_{42} = 0.0107\ h^{-1}$

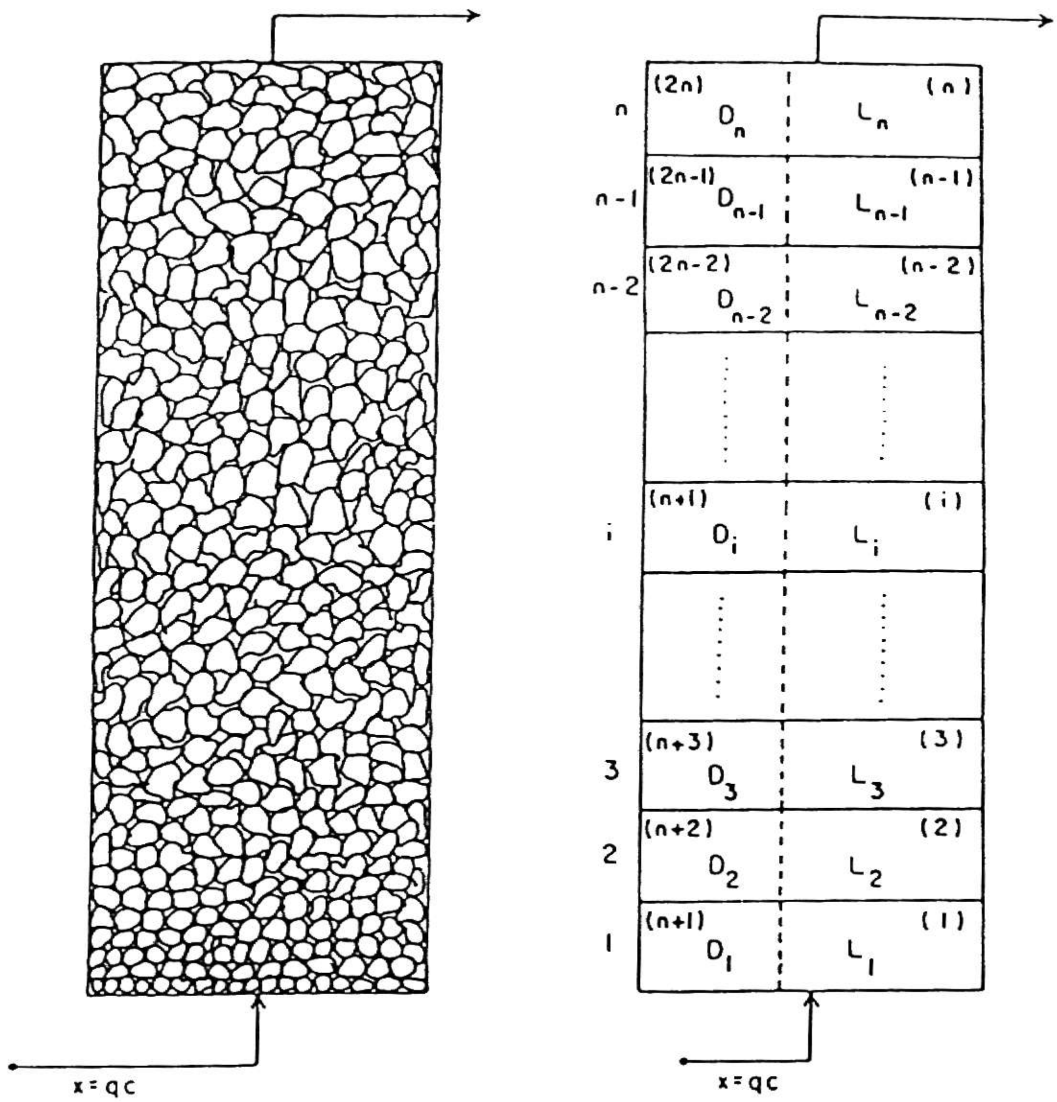

Figure 1. Schematic diagram of a deep-bed filter represented by a n-compartment model.

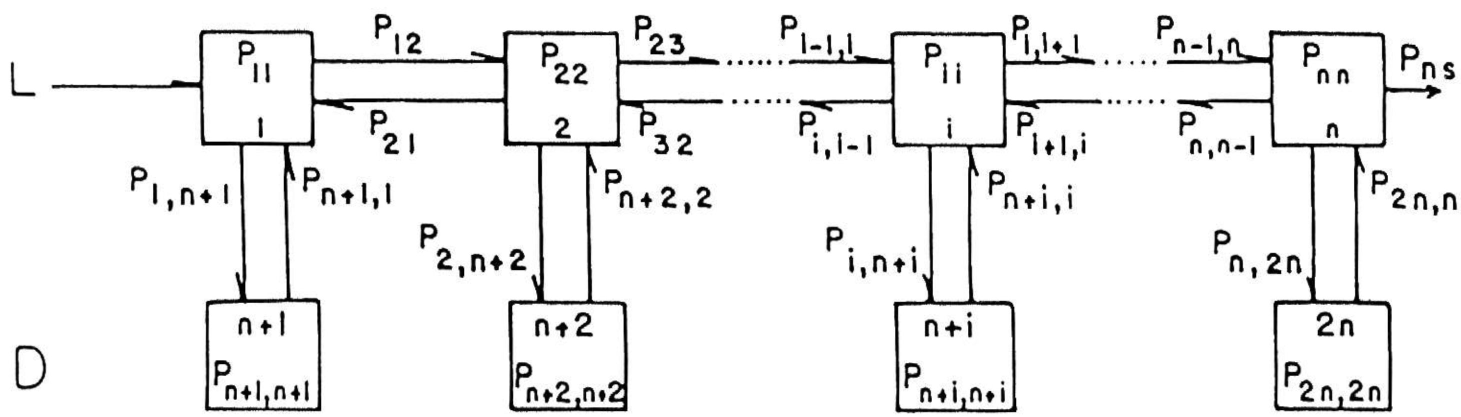

Figure 2. Transition diagram for a deep-bed filtration process.

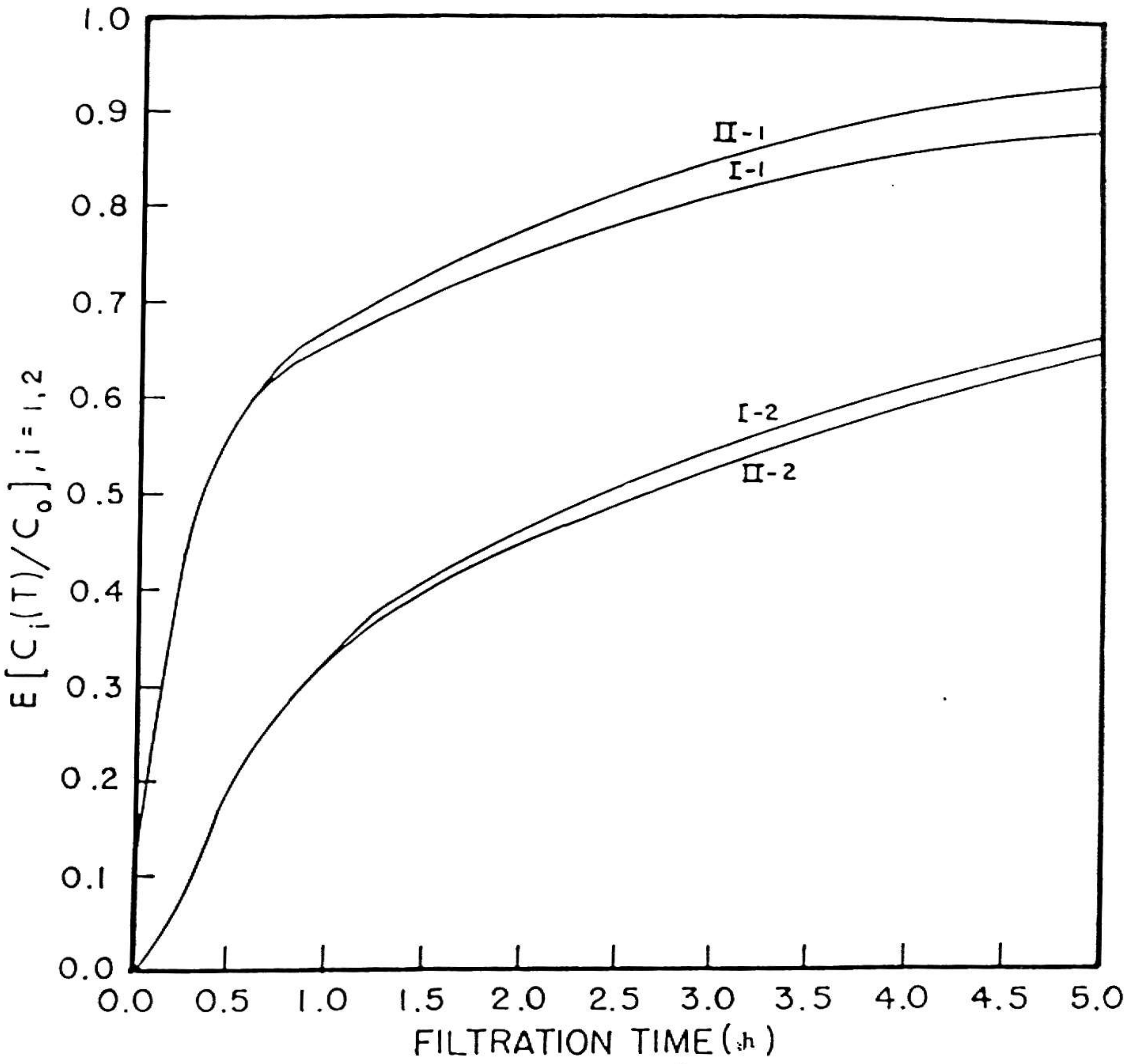

Figure 3. Simulation of the concentration dynamics of filtrates sampled from a deep-bed filter which is divided into two compartments with the following parameters to demonstrate the backmixing effect.

I : $m_{12} = 3.0h^{-1}$, $m_{13} = 2.0h^{-1}$, $m_{21} = 0.0h^{-1}$, $m_{24} = 1.0h^{-1}$,
$m_{31} = 0.5h^{-1}$, $m_{42} = 0.25h^{-1}$, $\mu_2 = 1.5h^{-1}$.

II: $m_{12} = 3.0h^{-1}$, $m_{13} = 2.0h^{-1}$, $m_{21} = 0.15h^{-1}$, $m_{24} = 1.0h^{-1}$,
$m_{31} = 0.5h^{-1}$, $m_{42} = 0.25h^{-1}$, $\mu_2 = 1.5h^{-1}$

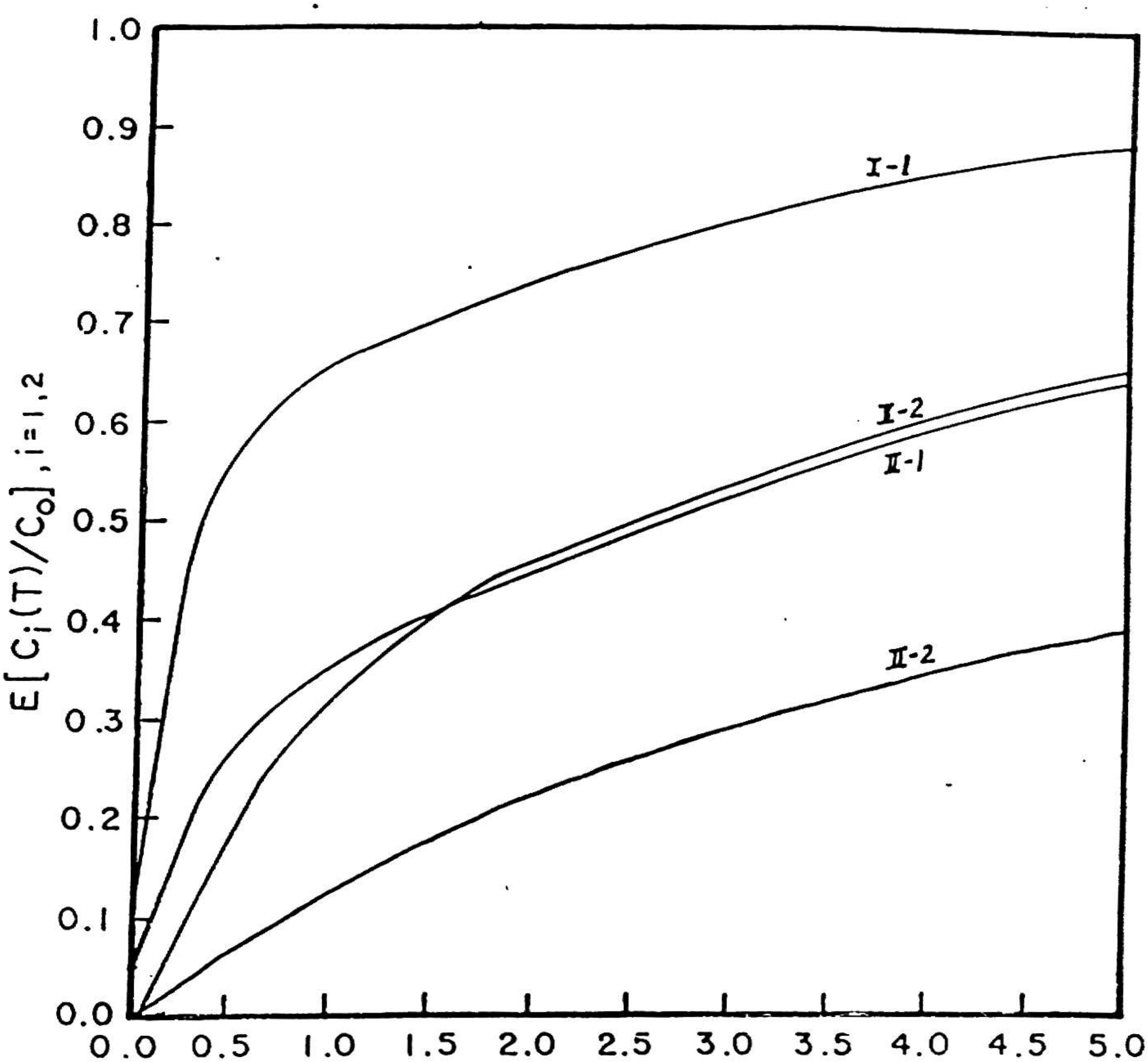

Figure 4. Simulation of the concentration dynamics of filtrates sampled from a deep-bed filter which is divided into two compartments with the following parameters to demonstrate the exit effect.

I : $m_{12} = 3.0h^{-1}$, $m_{13} = 2.0h^{-1}$, $m_{21} = 0.0h^{-1}$, $m_{24} = 1.0h^{-1}$, $m_{31} = 0.5h^{-1}$, $m_{42} = 0.25h^{-1}$, $\mu_2 = 1.5h^{-1}$.

II: $m_{12} = 1.0h^{-1}$, $m_{13} = 2.0h^{-1}$, $m_{21} = 0.0h^{-1}$, $m_{24} = 1.0h^{-1}$, $m_{31} = 0.5h^{-1}$, $m_{42} = 0.25h^{-1}$, $\mu_2 = 1.0h^{-1}$.

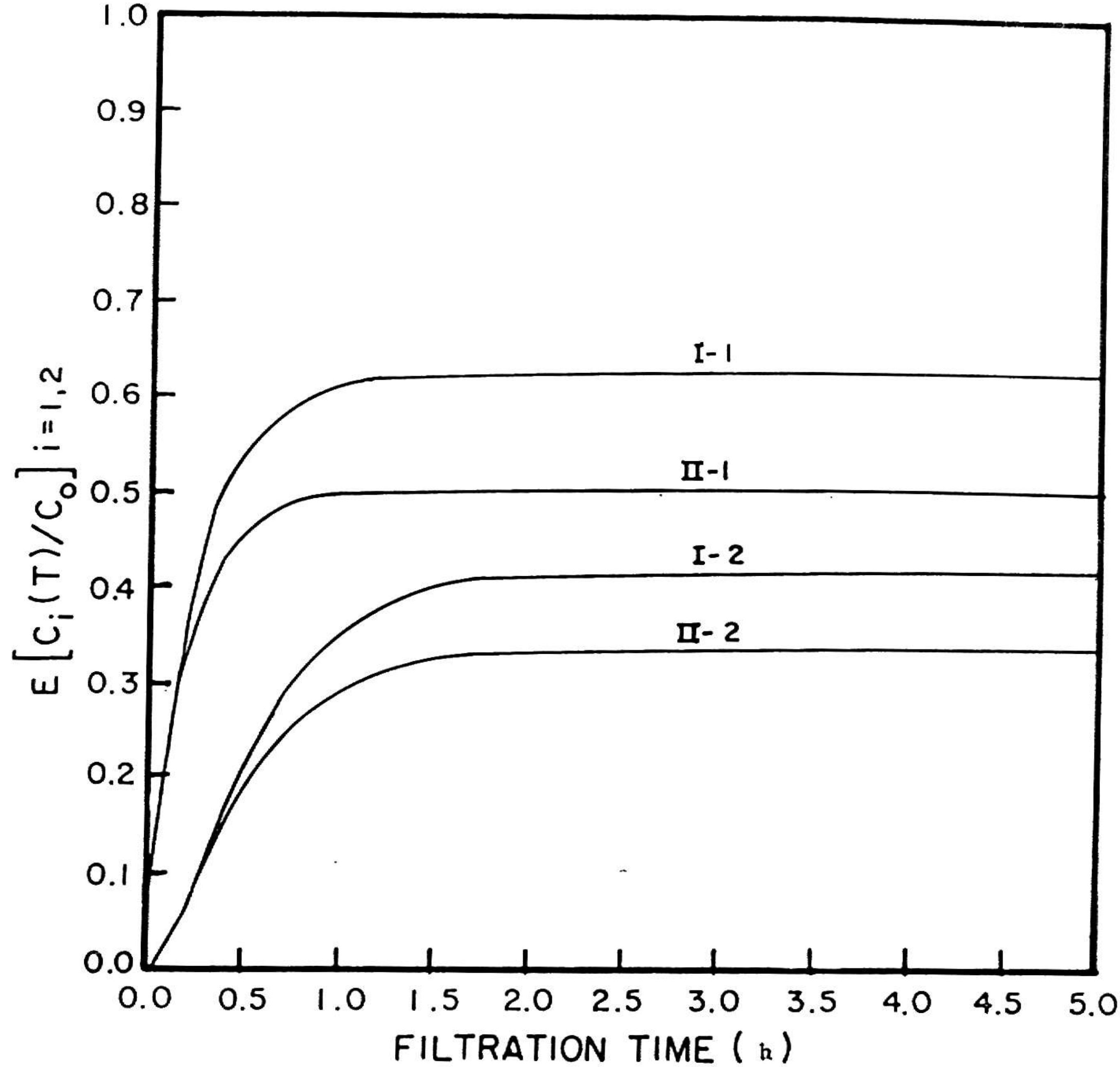

Figure 5. Simulation of concentration dynamics of filtrates sampled from a deep-bed filter which is divided into two compartments with the following parameters to show the characteristics of the filter bed with absorbing solid media.

I : $m_{12} = 2.5h^{-1}$, $m_{13} = 1.5h^{-1}$, $m_{24} = 1.0h^{-1}$, $\mu_2 = 2.0h^{-1}$,

$m_{21} = m_{31} = m_{42} = 0$.

II: $m_{12} = 2.5h^{-1}$, $m_{13} = 2.5h^{-1}$, $m_{24} = 1.0h^{-1}$, $\mu_2 = 2.0h^{-1}$,

$m_{21} = m_{31} = m_{42} = 0$.

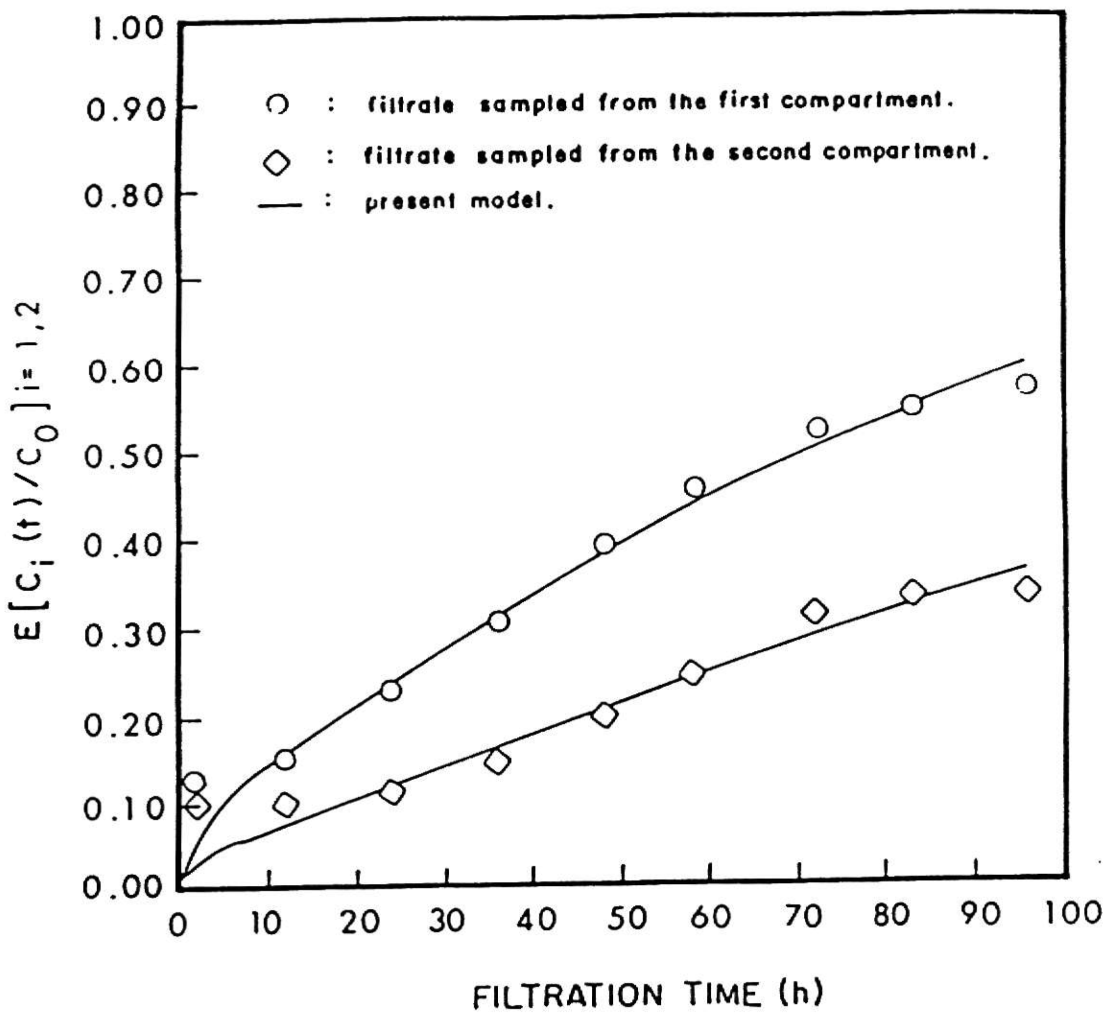

Figure 6. Fitting the present model to Eliassen's data (1935); sand diameter (0.051 cm), bed depth (60 cm), flow rate (0.136 cm/sec), hydrous ferric floc suspension (dia., 0.00124 cm; conc., 50 x 10^{-4} vol.%), 2 compartments.

Run 6:

$m_{12} = 29.677\ h^{-1}$, $m_{13} = 436.600\ h^{-1}$, $m_{31} = 0.1385\ h^{-1}$,

$\mu_2 = 16.713\ h^{-1}$, $m_{24} = 18.432\ h^{-1}$, $m_{42} = 0.0107\ h^{-1}$.

NOMENCLATURE

B_{rj}	=	defined in Eqs. 11 and 12
C	=	particle concentration of suspension
D_i	=	solid phase of compartment i
E[ ]	=	expected value of a random variable
$\underline{G}$	=	defined in Eq. 13
L_i	=	liquid phase of compartment i
$\underline{M}$	=	matrix of the intensity functions
m_{ij}	=	intensity function of a Markov process
$\underline{P}$	=	matrix of the transition probabilities $[p_{ij}]$
p_{ij}	=	transition probability
$\underline{Q}$	=	defined in Eq. 11
q	=	volumetric flow rate of suspension
S_i	=	states of a Markov process
t	=	time
V	=	volume of effluent collected
Var[ ]	=	variance of a randome variable
X	=	number of particles entering the bed per unit time
Y_i	=	random variable representing the number of particles in state i
y_i	=	observed value of Y_i
ρ	=	eigenvalue of matrix $\underline{M}$