COMMUNICATIONS TO THE EDITOR

A Markov Chain Model of a Packed Bed

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In an earlier contribution to this journal Schmalzer and Hoelscher (1971) presented a stochastic model of a packed bed and discussed the consequences on mixing and mass transfer. In the model it was assumed that each packet of fluid (or a particle) has three velocity states $\pm$, v, and '0'. The model then related the movement of the packet of fluid to a random walk problem in which the transition probabilities in the velocity space are appropriately chosen. The time parameter has been assumed to be discrete. It appears that most of the general features of mixing and mass transfer can be explained on the basis of this simple and elegant model. In view of the success of the model it is considered worthwhile to present a slightly improved version of the continuous Markov chain model which is expected to bring out some additional features of the underlying process. In fact a similar model with only two states $\pm v$ has been used in neutron transport problems (Bellman et al., 1958). The object of this note is to demonstrate the possibility of explicitly arriving at the residence time distribution corresponding to this model.

The problem will be treated as one-dimensional, the corresponding parameter x denoting the length of the bed traversed by the fluid packet during a time interval of duration t. It is assumed that at time $t = 0$ the fluid packet is just entering the bed (corresponding to $x = 0$) with propensity to move to the right with a velocity v. It is further assumed that the probability the fluid packet found to be in a velocity state i ($i = +, 0$ and $-$ standing respectively for the velocities $+ v$, 0 and $- v$) at time t jumps to a velocity ($i \neq j$) in the time interval $(t, t + \Delta)$ with probability $a_{ij}\Delta$ where Δ is infinitesimally small and positive; the probability of its continuance in the state i being

$$1 - \sum_{\substack{j \\ (i \neq j)}} a_{ij}\Delta$$

which is positive by virtue of Δ being an infinitesimal positive quantity. Thus the model corresponds to a purely discontinuous stochastic process of the Feller-Kolmogorov type [see, for example, Gnedenke (1969)]. In a preliminary discussion of this type, it is reasonable to take a_{ij}'s to be constants. Let $\pi_i(x, t)$ denote the probability that a fluid packet emerges at time t with its velocity characterized by a state i after traversing a total thickness x of the packed bed. The main quantities of interest are the functions $\pi_+(L, t)$ and $\pi_-(L, t)$, since these correspond to the probability of emergence of the fluid packet confined to $(0, L)$ (the volume corresponding to) from the right end and left end respectively. To determine these quantities we use the invariant imbedding technique (Bellman et al., 1958) and determine the functions $\pi_i(x, t)$. Explicitly we imbed the process corresponding to the time interval $(0, t)$ into a class of processes corresponding to the interval $(0, t + \Delta)$ with Δ arbitrary. By allowing Δ to take arbitrarily small values, we can obtain differential equations governing the functions $\pi_i(x, t)$ from which the required information can be extracted.

The probability that the particle emerges with a velocity $+v$ after traversing a distance x of the packed bed at time $t + \Delta$ arises from three mutually exclusive possibilities. First, the particle may emerge with a velocity $+v$ without undergoing any change in its velocity state in the time interval $(t, t + \Delta)$, the probability for this event being $(1 - a_{+-}\Delta - a_{+0}\Delta)\, \pi_+(x - v\Delta, t)$. Second, the particle is moving with velocity $-v$ at time t and therefore found to the right of x undergoes a transition from $-v$ to $+v$ during the time interval $(t, t + \Delta)$. The probability for this event is $a_{-+}\Delta\, \pi_-(x, t) + 0(\Delta)$. The last possibility corresponds to the particle being found stationary (that is, with a velocity equal to '0' at time t) undergoes a change in its velocity state from 0 to $+v$. The probability for this event is given by $a_{0+}\Delta\, \pi_0(x, t) + 0(\Delta)$. Thus adding all these possibilities we obtain

$$\pi_+(x, t + \Delta) = (1 - a_{++}\Delta)\, \pi_+(x - v\Delta, t) + a_{-+}\Delta\, \pi_-(x, t) + a_{0+}\Delta\, \pi_0(x, t) + 0(\Delta) \quad (1a)$$

where

$$a_{++} = a_{+-} + a_{+0}\,. \quad (1b)$$

In a similar manner, we obtain

$$\pi_-(x, t + \Delta) = (1 - a_{--}\Delta)\, \pi_-(x + v\Delta, t) + a_{+-}\Delta\, \pi_+(x, t) + a_{0-}\Delta\, \pi_0(x, t) + 0(\Delta) \quad (1c)$$

$$\pi_0(x, t + \Delta) = (1 - a_{00}\Delta)\,\pi_0(x, t) + a_{+0}\Delta\,\pi_+(x, t) + a_{-0}\Delta\,\pi_-(x, t) + 0(\Delta) \quad (1d)$$

where

$$a_{--} = a_{-+} + a_{-0}$$
$$a_{00} = a_{0+} + a_{0-} \quad (1e)$$

On proceeding to the limit as Δ tends to zero, we obtain

$$\frac{\partial \pi_+(x,t)}{\partial t} + v\frac{\partial \pi_+(x,t)}{\partial x} = -a_{++}\,\pi_+(x,t) + a_{-+}\,\pi_-(x,t) + a_{0+}\,\pi_0(x,t) \quad (2a)$$

$$\frac{\partial \pi_-(x,t)}{\partial t} - v\frac{\partial \pi_-(x,t)}{\partial x} = -a_{--}\,\pi_-(x,t) + a_{+-}\,\pi_+(x,t) + a_{0-}\,\pi_0(x,t) \quad (2b)$$

$$\frac{\partial \pi_0(x,t)}{\partial t} = -a_{00}\,\pi_0(x,t) + a_{+0}\,\pi_+(x,t) + a_{-0}\,\pi_-(x,t) \quad (2c)$$

Next we proceed to the solution of the Equations (2a) and (2b). Defining the Laplace transform of $\pi_i(x, t)$ as

$$\pi_i^*(x, s) = \int_0^\infty \pi_i(x, t)\, e^{-st}\, dt \quad i = +, - \text{ and } 0 \quad (3)$$

we can solve the above equations subject to the initial conditions

$$\pi_+(x, 0) = 0 \quad \pi_-(x, 0) = 0 \quad x > 0 \quad (4)$$

and boundary conditions

$$\pi_+(x,t) = 1 \quad \text{only at } x = 0, \quad t = 0$$
$$= 0 \quad \text{for} \quad x = 0 \quad t > 0 \quad (5)$$

$$\pi_-(x, t) = 0 \quad \text{at} \quad x = L \quad \text{for all } t. \quad (6)$$

The initial and boundary conditions correspond to the physical situation that at time $t = 0$ a particle (a fluid packed) enters the bed at $x = 0$ (from left) so that the entire contribution to the probability comes from $x = 0$. Equation (4) implies the absence of the particle at any other point in the bed. Equation (5) incorporates the boundary condition corresponding to the presence of the particle at $t = 0$ together with the condition that no other particle is injected into the bed subsequent to $t = 0$. Equation (6) on the other hand ensures that no other particle is injected into the bed at any time from the right hand end at $x = L$. Putting $v = 1$, using (4) after simplification we obtain the matrix equation as

$$\frac{\partial}{\partial x}\begin{bmatrix} \pi_+^*(x,s) \\ \pi_-^*(x,s) \end{bmatrix} = \begin{bmatrix} -(s + a_{++}) + \dfrac{a_{0+}a_{+0}}{s + a_{00}} & -a_{-+} + \dfrac{a_{0+}a_{-0}}{s + a_{00}} \\ -a_{+-} - \dfrac{a_{0-}a_{+0}}{s + a_{00}} & (s + a_{--}) + \dfrac{a_{0-}a_{-0}}{s + a_{00}} \end{bmatrix} \begin{bmatrix} \pi_+^*(x,s) \\ \pi_-^*(x,s) \end{bmatrix} \quad (7)$$

We can solve these equations by assigning suitable values to a_{ij}'s and obtain explicit expressions for $\pi_+^*(L, 0)$ and $\pi_-^*(0, 0)$ which are of practical interest. The function $\pi_+^*(L, 0)$ has an interesting property. It can be interpreted as the probability that it emerges out of the bed of extent L. Likewise $\pi_-^*(0, 0)$ represents the probability that the particle emerges out of bed by backflow. In addition to these, mean residence time for any finite t can also be calculated.

SIMPLE MODELS

The simplest model is obtained by taking the transition probabilities as constants each being equal to 1/3. Equation (7) reduces to

$$\frac{\partial}{\partial y}\begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ \dfrac{-3s}{3s+2} & 0 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} \quad (8)$$

where

$$p_1 = \pi_+^*(x, s) + \pi_-^*(x, s) \quad (9a)$$

$$p_2 = \pi_+^*(x, s) - \pi_-^*(x, s) \quad (9b)$$

and

$$y = x(s + 1)\,.$$

For $s = 0$, we obtain the explicit expressions for the forward and backward transition probabilities as

$$\pi_+^*(L, 0) = \frac{2}{L + 2} \quad (10a)$$

$$\pi_-^*(0, 0) = \frac{L}{L + 2} \quad (10b)$$

The general solutions for $\pi_+^*(x, s)$ and $\pi_-^*(x, s)$ can be found after some calculations as

$$\pi_+^*(x, s) = \frac{1}{A}\left[(1 + \lambda)^2 e^{-\lambda x(s+1)} - (1 - \lambda)^2 e^{-2\lambda L + \lambda x(s+1)}\right] \quad (11a)$$

$$\pi_-^*(x, s) = \frac{1}{A}\left[(1 - \lambda^2)\, e^{-\lambda x(s+1)} - (1 - \lambda^2)\, e^{-\lambda(2L - x(s+1))}\right] \quad (11b)$$

where

$$A = (1 + \lambda)^2 - (1 - \lambda)^2 e^{-2L\lambda} \quad \text{and} \quad \lambda^2 = \frac{3s}{3s + 2}.$$

Putting $s = 0$ and $x = L$ and $s = 0$, $x = 0$ respectively in (11a) and (11b) and applying L'Hospital's rule, we recover the forward and backward transition probabilities. The residence time density corresponding to the bed of length L is defined by

$$f(L, t) = \pi_+(L, t) + \pi_-(0, t) \quad (12)$$

When the fluid is flowing through the bed, some particles after spending random time in the bed may come out of the end $x = L$ or some particles will come out of the end $x = 0$ by backflow. The probability density function $f(L, t)$ governs both the cases. The quantity $f(L, t)dt$ has an alternative interpretation; it denotes the probability that the particle leaves the bed between t and $t + dt$. Since any particle after leaving the bed cannot re-enter, $f(L, t)$ simply denotes the probability density function governing the residence time in the bed. If we define $f(L)$ by

$$f(L) = \int_0^\infty t\,\pi_+(L, t)dt + \int_0^\infty t\,\pi_-(0, t)dt \quad (13)$$

we note that $f(L)$ represents the expected time spent by the particle in the bed and can therefore be identified with the mean residence time of the particle. The mean residence time can be readily obtained from the Laplace transform solution given by Equation (12)

$$f(L) = (3/2)\,L \qquad (14)$$

Next, we consider another simple model where the packets have a large propensity to move towards the right and have a small propensity to move left or become stationary. We can assign suitable values to a_{ij}'s to satisfy the above conditions.

For instance we can specify the choice by

$$a_{ij} = 2/3\ (i \neq j,\quad i = -v, 0 \quad j = +v) \qquad (15)$$
$$a_{ji} = 1/6$$

The probability of emergency in forward and backward directions are given by

$$\pi_+{}^*(L, 0) = \frac{3e^{(3/5)L}}{4e^{(3/5)L} - 1} \qquad (16)$$

and

$$\pi_-{}^*(0, 0) = \frac{e^{(3/5)L} - 1}{4e^{(3/5)L} - 1}$$

The explicit solutions for $\pi_+{}^*(x, s)$ and $\pi_-{}^*(x, s)$ are obtained as

$$\pi_+{}^*(x, s) = \frac{1}{A}\,[(\lambda_1 + 6s + 1)\, e^{+\lambda_2 \alpha x} - (\lambda_2 + 6s + 1)\, e^{(\lambda_2 - \lambda_1)L\alpha + \lambda_1 \alpha x}] \qquad (17)$$

$$\pi_-{}^*(x, s) = \frac{1}{4A}\,[(\lambda_1 + 6s + 1)(\lambda_2 + 6s + 1)\, e^{\lambda_2 \alpha x} - (\lambda_2 + 6s + 1)(\lambda_1 + 6s + 1)\, e^{(\lambda_2 - \lambda_1)L\alpha + \lambda_1 \alpha x}]$$

where

$$A = (\lambda_1 + 6s + 1) - (\lambda_2 + 6s + 1)\, e^{(\lambda_2 - \lambda_1)L\alpha} \qquad (18)$$

and

$$\alpha = \frac{(s + 1)}{6s + 5},$$

$$\lambda_1 = \frac{1}{2}\,[3 + [4(6s + 1)(6s + 4) - 7]^{1/2}]$$

$$\lambda_2 = \frac{1}{2}\,[3 - [4(6s + 1)(6s + 4) - 7]^{1/2}]$$

In this case, the mean residence time is found to be

$$f(L) = \frac{1}{(-e^{-(3/5)L} + 4)^2}\,[A + e^{-(3/5)L}(B + DL) + e^{-(6/5)L}(C + EL) + FL] \qquad (19)$$

where

$$A = \frac{-1552}{100} \qquad C = \frac{-26}{4}$$
$$B = \frac{5038}{100} \qquad E = \frac{-406}{25}$$
$$D = \frac{620}{125} \qquad F = \frac{2412}{25}$$

Finally, we study the behavior of the fluid packets when the transition probabilities depend on the individual states and are characterized by a large propensity to move forward. For purpose of illustration, we make the following choice of the constants.

$$a_{-+} = .98,\quad a_{0+} = .89,\quad a_{-0} = .015,\quad a_{0-} = .01$$
$$a_{+-} = .01,\quad \text{and} \quad a_{+0} = .03\,. \qquad (20)$$

With these transition probabilities, the explicit expression for the forward and backward transition probabilities for an infinite period of time are given by

$$\left.\begin{aligned} \pi_+{}^*(L, 0) &= \frac{99e^{.98L}}{100e^{.98L} - 1} \\ \pi_-{}^*(0, 0) &= \frac{e^{.98L} - 1}{100e^{.98L} - 1} \end{aligned}\right\} \qquad (21)$$

while the Laplace transform solution are given by

$$\pi_+{}^*(x, s) = \frac{1}{A}\,[(\lambda_1 + s^2 + .94s + .01)\, e^{\lambda_2 \alpha x} - (\lambda_2 + s^2 + .94s + .01)\, e^{(\lambda_2 - \lambda_1)L\alpha + \lambda_1 \alpha x}] \qquad (22)$$

$$\pi_-{}^*(x, s) = \frac{1}{A}\,[(\lambda_1 + s^2 + .94s + .01)$$
$$(\lambda_2 + s^2 + .94s + .01)\, e^{\lambda_2 \alpha x} - (\lambda_1 + s^2 + .94s + .01)$$
$$(\lambda_2 + s^2 + .94s + .01)\, e^{(\lambda_2 - \lambda_1)L\alpha + \lambda_1 \alpha x}]$$

where

$$A = (\lambda_1 + s^2 + .94s + .01) - (\lambda_2 + s^2 + .94s + .01)e^{(\lambda_2 - \lambda_1)L\alpha}$$

and

$$\alpha = \frac{1}{s + .9},$$

$$\lambda_1 = \frac{1}{2}\,[.95s + .89 + [(.95s + .89)^2 + 4\{(s^2 + .94s + .01)(s^2 + 1.89s + .9) - (.98s + .89)(.01s + .01)\}]^{1/2}]$$

$$\lambda_2 = \frac{1}{2}\,[.95s + .89 - [(.95s + .89)^2 + 4\{(s^2 + .94s + .01)(s^2 + 1.89s + .9) - (.98s + .89)(.01s + .01)\}]^{1/2}]$$

Putting $s = 0$ and choosing $x = 0$ and L, we can cover Equation (21) from (22)

The mean residence time is given by

$$f(L) = \frac{1}{(.9 - .01\, e^{-.98L})^2}\,[AL + e^{-.98L}\,(BL + C) + e^{-1.96L}\,(DL + E)] \qquad (23)$$

where

$$A = 2.115,\quad B = .0504,\quad C = -.14,$$
$$D = .0008,\quad E = .0269\,.$$

It is hoped that these results will be useful in interpretation of experiments. It is possible to obtain an estimate for the standard deviation of the residence time. Numerical work relating to the inversion of the Laplace transform is in progress.

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