

A MODEL OF THE COUNTER-CURRENT FLOW OF THE DISPERSED AND THE CONTINUOUS PHASE. MONODISPERSED SYSTEMS

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Two discretized stochastic models have been proposed in the paper of the counter-current flow of the dispersed and the continuous phase: A simulation model and a probabilistic model of the Markov's chain type. A comparison of both models has been made and their relation to the differential model of van de Vusse has been established.

Counter-current flow of the dispersed and the continuous phase constitutes often an important part of the phenomena in the continuously operated contact apparatuses. Mutual motion of the phases takes place through the gravity or centrifugal forces. The principal phenomenon in these apparatuses is mass transfer eventually accompanied by chemical reactions. The rates of both mass transfer and chemical reactions are generally functions of time and position and it is thus apparent that the knowledge of the distribution of those quantities that affect the transfer rates will be of primary importance. These quantities are mainly concentration of the dispersed phase and in case of polydispersed systems also functions describing the particle size distribution and eventually also the distribution of their residence time within the apparatus. Because the flow in contactors is mostly turbulent the counter-current flow of both the continuous and the dispersed phase is being perturbed. The distribution functions thus become random functions and statistical characteristics enter the description of the process in question.

It has been found experimentally¹⁻⁴ that the hold-up of the dispersed phase in counter-current extraction columns is not constant along the height of the column. There may be several causes of this finding. Van de Vusse⁵ has shown that the hold-up of the dispersed phase may be expected to decrease steadily in the direction of its flow if there is a fluctuation velocity component superimposed on the falling velocity of a monodispersed system. According to the model proposed by Rod⁶, which combines the effect of axial dispersion and the decrease of the falling velocity of droplets due to their gradual dispergation, profiles of the hold-up may exhibit maxima within the column as has been confirmed by experimental observation³.

This work is an initial study of the hydrodynamics of the counter-current flow of the dispersed and the continuous phase aimed at the general case when both axial mixing of the dispersion and splitting and coalescence of the droplets exist. The models to be proposed here were formulated for monodispersed systems but they are expected to find full use in application to polydispersed systems. Two stagewise models corresponding to the differential model due to van de Vusse⁵ have been proposed. The latter can be described as follows: Starting from an instant $t = 0$ a steady flow of a monodispersion of density q is fed into a column. The dispersion moves through the column against the flow of the continuous phase while neither splitting nor coalescence of the droplets takes place. The dispersion moves in plug flow at the velocity v related to the wall of the column. Superimposed to this convective flow there is axial dispersion, characterized by the dispersion coefficient D relating to the gradient of particle concentration $\partial n/\partial y$. At the point $y = L$, where the continuous phase is fed, the velocity of the droplets increases to a value k . At $y = L'$ the axial dispersion decays. The effect of particle concentration on the velocity of the convective flow as well as axial dispersion is neglected. This makes D , v and k constants. The pertaining differential equations and boundary conditions read

$$\partial n/\partial t = D\partial^2 n/\partial y^2 - v\partial n/\partial y; \quad 0 < y \leq L \quad (1)$$

$$\partial n/\partial t = D\partial^2 n/\partial y^2 - k\partial n/\partial y; \quad L \leq y \leq L' \quad (2)$$

$$\partial n/\partial t = -k\partial n/\partial y; \quad L' \leq y \quad (3)$$

$$t = 0; \quad n = 0; \quad (4)$$

$$t > 0; \quad y = 0; \quad vn - D\partial n/\partial y = q \quad (5)$$

$$y = L; \quad n_{L-} = n_{L+}; \quad \left(vn - D \frac{\partial n}{\partial y} \right)_{L-} = \left(kn - D \frac{\partial n}{\partial y} \right)_{L+} \quad (6)$$

$$y = L'; \quad n_{L'-} = n_{L'+}; \quad \left(kn - D \frac{\partial n}{\partial y} \right)_{L'-} = kn_{L'+}. \quad (7)$$

Stochastic Model

This model views the column of unit cross-section as consisting of perfectly mixed stages of height Δl . At the instant $t = 0$ the first stage is fed by monodispersion at the rate q_0 particles per time increment Δt . The continuous phase is fed into the N_1 -th stage. Backmixing of the dispersed phase occurs between individual stages as a random process. This process vanishes starting from the stage N_2 . The spatial and

the time coordinate are discrete ($y_i = i \Delta l$; $t_j = j \Delta t$; $\Delta l, \Delta t = \text{const.}$; $i = 0, 1, 2, \dots$). In view of the random character of axial dispersion both the local instantaneous concentrations of the droplets in the column ($m_{i,j}/\Delta l$) and the density of the flow of the droplets at the exit of the column ($q_{N,j}$) are random variables.

The population balance of the i -th stage may be formulated as follows

$$m_{1,j} = [1 - (\frac{1}{2} + \delta_{1,j-1}) d_1 - \frac{1}{2}r_1 - f_1] m_{1,j-1} + q_0 + [\frac{1}{2} - \delta_{2,j-1}] d_1 + \frac{1}{2}r_1] m_{2,j-1} \quad (8)$$

$$m_{i,j} = (1 - d_1 - r_1 - f_1) m_{i,j-1} + [(\frac{1}{2} + \delta_{i-1,j-1}) d_1 + \frac{1}{2}r_1 + f_1] m_{i-1,j-1} + [(\frac{1}{2} - \delta_{i+1,j-1}) d_1 + \frac{1}{2}r_1] m_{i+1,j-1}; \quad 1 < i < N_1 \quad (9)$$

$$m_{N_1,j} = [1 - (\frac{1}{2} - \delta_{N_1,j-1}) d_1 - (\frac{1}{2} + \delta_{N_1,j-1}) d_2 - \frac{1}{2}r_1 - \frac{1}{2}r_2 - f_2] m_{N_1,j-1} + [(\frac{1}{2} + \delta_{N_1-1,j-1}) d_1 + \frac{1}{2}r_1 + f_1] m_{N_1-1,j-1} + [(\frac{1}{2} - \delta_{N_1+1,j-1}) d_2 + \frac{1}{2}r_2] m_{N_1+1,j-1}; \quad (10)$$

$$m_{i,j} = (1 - d_2 - r_2 - f_2) m_{i,j-1} + [(\frac{1}{2} + \delta_{i-1,j-1}) d_2 + \frac{1}{2}r_2 + f_2] m_{i-1,j-1} + [(\frac{1}{2} - \delta_{i+1,j-1}) d_1 + \frac{1}{2}r_1] m_{i+1,j-1}; \quad N_1 < i < N_2 \quad (11)$$

$$m_{N_2,j} = [1 - (\frac{1}{2} - \delta_{N_2,j-1}) d_2 - \frac{1}{2}r_2 - f_2] m_{N_2,j-1} + [(\frac{1}{2} + \delta_{N_2-1,j-1}) d_2 + \frac{1}{2}r_2 + f_2] m_{N_2-1,j-1}; \quad (12)$$

$$m_{i,j} = (1 - f_2) n_{i,j-1} + f_2 n_{i-1,j-1}; \quad N_2 < i; \quad (13)$$

$$m_{i,0} = 0; \quad 1 \leq i. \quad (14)$$

These balances contain three parameters d , r and f characterizing the rate of convective transport (f) and axial mixing (d , r) of the droplets. These parameters assume constant values over individual sections of the extractor. The parameter f represents the fractional number of the droplets in the i -th stage transported by convection into the $i + 1$ -th stage per time t . In case of counter-current flow f is positive. The stochastic character of axial mixing shows in the appropriate coefficient of back-mixing being composed of the constant ($r/2$) and the random ($\delta_{i,j}d$) component where $\delta_{i,j}$ is a random quantity with a uniform distribution $H(0, 1/2)$, i.e. the probability density

$$\pi(\delta) = \begin{cases} 1 & \text{for } -1/2 \leq \delta \leq 1/2 \\ 0 & \text{otherwise} \end{cases} \quad (15)$$

The dependent variable $m_{i,j}$ is clearly also a random function of integer variables i, j . The parameters d and r are non-negative and represent again the fractional number of droplets within the stage displaced during a single time increment. Owing the definitions of the parameters d, r and f as fractional amounts of droplets in a given stage which emerge during a given time increment from the stage we must require that

$$0 < d + r + f \leq 1. \quad (16)$$

In order that we may compare the stochastic with the deterministic model of van de Vusse we must implement certain modifications of Eqs (8)–(14): Firstly, we shall determine their expected values. This means that we replace the random variables by their expected values (means) and define new parameters

$$\begin{aligned} \bar{n}_{i,j} &\equiv E(m_{i,j}/\Delta l); \quad v \equiv f_1 \Delta l / \Delta t; \quad k \equiv f_2 \Delta l / \Delta t; \quad \bar{r}_1 \equiv (d_1 + r_1) / 2f_1; \\ \bar{r}_2 &\equiv (d + r_2) / 2f_2; \quad q \equiv q_0 / \Delta t. \\ (\bar{n}_{1,j} - n_{1,j-1}) / \Delta t &= q / \Delta l + [\bar{r}_1 \bar{n}_{2,j-1} - (1 + \bar{r}_1) \bar{n}_{1,j-1}] v / \Delta l; \end{aligned} \quad (17)$$

$$\begin{aligned} (\bar{n}_{i,j} - \bar{n}_{i,j-1}) / \Delta t &= [(1 + \bar{r}_1) \bar{n}_{i-1,j-1} + \bar{r}_1 \bar{n}_{i+1,j-1} - (1 + 2\bar{r}_1) \bar{n}_{i,j-1}] v / \Delta l; \\ &1 < i < N_1; \end{aligned} \quad (18)$$

$$\begin{aligned} (\bar{n}_{N_1,j} - \bar{n}_{N_1,j-1}) / \Delta t &= [(1 + \bar{r}_1) \bar{n}_{N_1-1,j-1} v + \bar{r}_2 \bar{n}_{N_1+1,j-1} k - \\ & - \bar{r}_1 \bar{n}_{N_1,j-1} v - (1 + \bar{r}_2) \bar{n}_{N_1,j-1} k] / \Delta l; \end{aligned} \quad (19)$$

$$\begin{aligned} (\bar{n}_{i,j} - \bar{n}_{i,j-1}) / \Delta t &= [(1 + \bar{r}_2) \bar{n}_{i-1,j-1} + \bar{r}_2 \bar{n}_{i+1,j-1} - \\ & - (1 + 2\bar{r}_2) \bar{n}_{i,j-1}] k / \Delta l; \quad N_1 < i < N_2; \end{aligned} \quad (20)$$

$$(\bar{n}_{N_2,j} - \bar{n}_{N_2,j-1}) / \Delta t = [(1 + \bar{r}_2) (\bar{n}_{N_2-1,j-1} - \bar{n}_{N_2,j-1})] k / \Delta l; \quad (21)$$

$$(\bar{n}_{i,j} - \bar{n}_{i,j-1}) / \Delta t = (\bar{n}_{i-1,j-1} - \bar{n}_{i,j-1}) k / \Delta l; \quad N_2 < i; \quad (22)$$

$$\bar{n}_{i,0} = 0; \quad 1 \leq i. \quad (23)$$

By arrangement of the above equations to a form analogous to the differential we finally obtain

$$\frac{\Delta \bar{n}_{i,j-1}}{\Delta t} = \left(\frac{1}{2} + \bar{r}_1\right) v \Delta l \frac{\Delta^2 \bar{n}_{i+1,i-1}}{(\Delta l)^2} - v \frac{\Delta \bar{n}_{i+1,i-1}}{\Delta l}; \quad 1 < i < N_1; \quad (24)$$

$$\frac{\Delta \bar{n}_{j,j-1}}{\Delta t} = \left(\frac{1}{2} + \bar{r}_2\right) k \Delta l \frac{\Delta^2 \bar{n}_{i+1,i-1}}{(\Delta l)^2} - k \frac{\Delta \bar{n}_{i+1,i-1}}{\Delta l}; \quad N_1 < i < N_2; \quad (25)$$

$$\frac{\Delta \bar{n}_{j,j-1}}{\Delta t} = -k \frac{\Delta \bar{n}_{i,i-1}}{\Delta l}; \quad N_2 < i; \quad (26)$$

$$\bar{n}_{i,0} = 0; \quad 1 \leq i; \quad (27)$$

$$v \bar{n}_{1+1/2} - \left(\frac{1}{2} + \bar{r}_1\right) v \Delta l \frac{\Delta \bar{n}_{2,1}}{\Delta l} = q - \Delta l \frac{\Delta \bar{n}_{j,j-1}}{\Delta t}; \quad i = 1; \quad (28)$$

$$\begin{aligned} & v \bar{n}_{N_1-1/2} - \left(\frac{1}{2} + \bar{r}_1\right) v \Delta l \frac{\Delta \bar{n}_{N_1, N_1-1}}{\Delta l} = \\ & = k \bar{n}_{N_1+1/2} - \left(\frac{1}{2} + \bar{r}_2\right) k \Delta l \frac{\Delta \bar{n}_{N_1+1, N_1}}{\Delta l} + \Delta l \frac{\Delta \bar{n}_{j,j-1}}{\Delta t}; \quad i = N_1; \quad (29) \end{aligned}$$

$$\begin{aligned} & k \bar{n}_{N_2-1/2} - \left(\frac{1}{2} + \bar{r}_2\right) k \Delta l \frac{\Delta \bar{n}_{N_2, N_2-1}}{\Delta l} = \\ & = k \bar{n}_{N_2, j-1} + \Delta l \frac{\Delta \bar{n}_{j,j-1}}{\Delta t}; \quad i = N_2. \quad (30) \end{aligned}$$

In these equations

$$\Delta \bar{n}_{j,j-1} = \bar{n}_{i,j} - \bar{n}_{i,j-1}; \quad \Delta^2 \bar{n}_{i+1,i-1} = \bar{n}_{i+1,j-1} - 2\bar{n}_{i,j-1} + \bar{n}_{i-1,j-1};$$

$$\Delta \bar{n}_{i+1,i-1} = (\bar{n}_{i+1,j-1} - \bar{n}_{i-1,j-1})/2;$$

$$\Delta \bar{n}_{i,i-1} = \bar{n}_{i,j-1} - \bar{n}_{i-1,j-1};$$

$$\Delta \bar{n}_{i+1,i} = \bar{n}_{i+1,j-1} - \bar{n}_{i,j-1};$$

$$\bar{n}_{i+1/2} = (\bar{n}_{i,j-1} + \bar{n}_{i+1,j-1})/2;$$

$$\bar{n}_{i-1/2} = (\bar{n}_{i-1,j-1} + \bar{n}_{i,j-1})/2.$$

It is obvious that Eqs (24)–(30) transform in the limit $\Delta t = 0$, $\Delta l = 0$ into Eqs (1)–(6). It must be noted that for a given intensity of axial mixing decreasing Δl causes necessarily corresponding growth of \bar{r} so as to keep the expression $(1/2 + r) u \Delta l$ constant (u corresponds to v or k). From the comparison we have the following equivalence

$$D = (1/2 + \bar{r}_1) v \Delta l = (1/2 + \bar{r}_2) k \Delta l. \quad (31)$$

The term $1/2$ in these expressions accounts for the fact that even for $\bar{r} = 0$ the system of ideal mixers of finite height Δl causes certain axial mixing. In the limit $\Delta l \rightarrow 0$, $\bar{r} \rightarrow \infty$ the influence of the mentioned term clearly vanishes.

From Eq. (31) and the definitions of the quantities appearing in it, it follows

$$d_1 + r_1 + f_1 = d_2 + r_2 + f_2. \quad (32)$$

On defining the Peclet numbers for the differential model as

$$\text{Pe}_1 = v \Delta l / D; \quad \text{Pe}_2 = k \Delta l / D \quad (33)$$

we have the following equivalences

$$\frac{1}{\text{Pe}_1} = \frac{1}{2} + \bar{r}_1; \quad \frac{1}{\text{Pe}_2} = \frac{1}{2} + \bar{r}_2. \quad (34)$$

A similar expression has been derived by Miyauchi and Vermeulen⁷ for steady state extraction with axial mixing. The characteristic length Δl in Eqs (31) and (33) may be thought of as the construction height of a stage of a stagewise extractor and the equivalence then pertains the application of the differential or stagewise model to the stagewise extractor. It is worth noting that in the balance of the first stage, Eq. (28), which is an analog of the boundary condition (5) of the differential model, an accumulation term appears due to the finite dimensions of the examined volume element.

The analogy of both models may thus be summarized in the following equations

$$\left. \begin{aligned} y \rightarrow i \Delta l; \quad \bar{n} \rightarrow E(m/\Delta l); \quad k \rightarrow f_2 \Delta l / \Delta t; \quad t \rightarrow j \Delta t; \quad v \rightarrow f_1 \Delta l / \Delta t; \\ D \rightarrow \left(\frac{1}{2} + \frac{d_1 + r_1}{2f_1} \right) v \Delta l = \left(\frac{1}{2} + \frac{d_2 + r_2}{2f_2} \right) k \Delta l; \\ q \rightarrow q_0 / \Delta t. \end{aligned} \right\} \quad (35)$$

Because the simulation model contains one more parameter than the differential model it is desirable to introduce one more relation between the parameters. A plausible alternative is

$$d_1/r_1 = d_2/r_2. \quad (36)$$

As the next step we determine the number of independent parameters of the stochastic model. For this purpose it is convenient to rewrite Eqs (24)–(30) into the

dimensionless form. Introducing a dimensionless concentration

$$v = \bar{n}/n_0; \quad n_0 = q/v = q_0/(f_1 \Delta l); \quad (37)$$

$$\frac{1}{f_1} \Delta v_{j,j-1} = \left(\frac{1}{2} + \bar{r}_1\right) \Delta^2 v_{i+1,i-1} - \Delta v_{i+1,i-1}; \quad 1 < i < N_1; \quad (38)$$

$$\frac{1}{f_1} \Delta v_{j,j-1} = \left(\frac{1}{2} + \bar{r}_2\right) \frac{f_2}{f_1} \Delta^2 v_{i+1,i-1} - \frac{f_2}{f_1} \Delta v_{i+1,i-1}; \quad N_1 < i < N_2; \quad (39)$$

$$\frac{1}{f_1} \Delta_{j,j-1} = -\frac{f_2}{f_1} \Delta v_{i,i-1}; \quad N_2 < i; \quad (40)$$

$$v_{i,0} = 0; \quad 1 \leq i; \quad (41)$$

$$\frac{1}{f_1} \Delta v_{j,j-1} = \left(\frac{1}{2} + \bar{r}_1\right) \Delta v_{2,1} + 1 - v_{1+1/2}; \quad i = 1; \quad (42)$$

$$\begin{aligned} \frac{1}{f_1} \Delta v_{j,j-1} = & -\left(\frac{1}{2} + \bar{r}_1\right) \Delta v_{N_1,N_1-1} + v_{N_1-1/2} + \\ & + \left(\frac{1}{2} + \bar{r}_2\right) \frac{f_2}{f_1} \Delta v_{N_1+1,N_1} - \frac{f_1}{f_2} v_{N_1+1/2}; \quad i = N_1; \end{aligned} \quad (43)$$

$$\frac{1}{f_1} \Delta v_{j,j-1} = -\left(\frac{1}{2} + \bar{r}_2\right) \frac{f_2}{f_1} \Delta v_{N_2,N_2-1} + \frac{f_2}{f_1} v_{N_2-1/2} - \frac{f_2}{f_1} v_{N_2}; \quad i = N_2. \quad (44)$$

As independent parameters we may thus choose *e.g.* $f_1, f_2/f_1, d/r, d + r + f, N_1, N_2/N_1$.

Probabilistic Model

The difference equations for the expected values (means) of the previous model may be assigned their probabilistic meanings. Let us term the appearance of a droplet in the i -th stage of the apparatus by its state $X = i$ and define the family of the states ($i = 1, 2, \dots, N + 1$). The state of the droplet is a function of time which is defined as a discrete variable ($j = 1, 2, \dots$); the sequence of these states in time constitutes the examined process. The probability that a droplet appears in time j in the state X is designated as $x(j)$. Further, p_{ik} is the probability of the transition of the droplet from state i into state k over a single time increment ($k = 1, 2, \dots, N + 1$). With

respect to Eqs (17)–(23) the process in question is one of Markov. This means that the state at a time j depends only on the state at the time $j - 1$ and not on the earlier states. Because the independent variables are discrete we are dealing with the so called Markov's chain⁸.

The principal assumptions of the stochastic model are following: A1) The motion of an individual droplet is independent of the motion of the rest of the particles. A2) The mechanisms giving rise to individual types of droplet's displacements are independent. A3) Transitions during a single time increment occur only between neighbouring states. A4) The probability of a transition is independent of time.

From the assumptions A1–A3 it follows that the flow of droplets through the apparatus can be depicted as a superimposed motion of individual droplets or groups of droplets entering the equipment at the same time increment. Further, the probability of the resulting displacement of a droplet in a given direction equals the sum of the probabilities of partial displacements in this direction induced by individual transport mechanisms.

As follows from Eqs (17)–(22) the probabilities of the transition may be arranged into a tridiagonal square transition matrix whose rows represent the original state of the droplet and the columns the state in which the droplet with the given probability enters during the time increment. In accord with the assumption A4 the matrix is stationary.

In order that the described Markov's process be fully analogous to the averaged stochastic process described previously we shall introduce conditions enabling individual probabilities of the transition to be determined:

C1: The droplets enter only the first stage and leave only from the N -th stage. The droplets that have left the system do not reenter.

C2: In the section between the first and the N_1 -th stage the probability of the transition forward is $[(d_1 + r_1)/2] + f_1$ and back $(d_1 + r_1)/2$. In the section between $N_1 + 1$ and N_2 these probabilities are $[(d_2 + r_2)/2] + f_2$ and $(d_2 + r_2)/2$. In the section between $N_2 + 1$ and N there can be only forward transitions with the probability f_2 . According to C1 the transition matrix has the rank of $N + 1$ (the droplet leaving the stage N enters the auxiliary "absorption stage" $N + 1$ to remain there). Transition matrices possessing this property are called irreducible.

Let us designate the transition matrix by

$$\mathbf{P} \equiv \{p_{ik}\}; \quad i, k = 1, \dots, N + 1. \quad (45)$$

The diagonal elements ($i = k$) of the matrix represent the probability that the droplet remains during the time increment in the original state. Thus we have

$$\sum_k p_{ik} = 1; \quad k = 1, \dots, N + 1 \quad (46)$$

According to C1 and C2 we may write

$$\left. \begin{aligned} p_{i,i-1} &= (d_1 + r_1)/2; \\ p_{i,i+1} &= [(d_1 + r_1)/2] + f_1; \\ p_{i,i} &= 1 - (d_1 + r_1 + f_1); \\ p_{i,k} &= 0; \quad k \neq i-1, i, i+1; \end{aligned} \right\} \text{for } 1 < i \leq N_1 \quad (47)$$

$$\left. \begin{aligned} p_{i,i-1} &= (d_2 + r_2)/2; \\ p_{i,i+1} &= [(d_2 + r_2)/2] + f_2 \\ p_{i,i} &= 1 - (d_2 + r_2 + f_2); \\ p_{i,k} &= 0; \quad k \neq i-1, i, i+1; \end{aligned} \right\} \text{for } N_1 < i \leq N_2 \quad (48)$$

$$\left. \begin{aligned} p_{i,i+1} &= f_2; \\ p_{i,i} &= 1 - f_2; \\ p_{i,k} &= 0; \quad k \neq i, i+1; \end{aligned} \right\} \text{for } N_2 < i \leq N \quad (49)$$

$$\left. \begin{aligned} p_{1,2} &= [(d_1 + r_1)/2] + f_1; \\ p_{1,1} &= 1 - [(d_1 + r_1)/2] - f_1; \\ p_{1,k} &= 0; \quad k \neq 1, 2; \end{aligned} \right\} \quad (50)$$

$$\left. \begin{aligned} p_{N_1, N_1-1} &= (d_1 + r_1)/2; \\ p_{N_1, N_1+1} &= [(d_2 + r_2)/2] + f_2; \\ p_{N_1, N_1} &= 1 - [(d_1 + r_1)/2] - [(d_2 + r_2)/2] - f_2; \\ p_{N,k} &= 0; \quad k \neq N_1 - 1, N_1, N_1 + 1; \end{aligned} \right\} \quad (51)$$

$$\left. \begin{aligned} p_{N_2, N_2-1} &= (d_2 + r_2)/2; \\ p_{N_2, N_2+1} &= f_2; \\ p_{N_2, N_2} &= 1 - [(d_2 + r_2)/2] - f_2; \\ p_{N_2, k} &= 0; \quad k \neq N_2 - 1, N_2, N_2 + 1; \end{aligned} \right\} \quad (52)$$

$$p_{N+1, N+1} = 1. \quad (53)$$

The initial distribution of the particles in the system is given by the column vector as

$$\mathbf{p}(0) \equiv \{p(0)_i\}; \quad i = 1, \dots, N + 1, \quad (54)$$

where p_{0i} is the probability that the entering particle assumes the state i .

Thus

$$\begin{aligned} p(0)_1 &= 1; \\ p(0)_i &= 0; \quad i \neq 1. \end{aligned} \quad (55)$$

In accord with the theory of Markov's chains the probability of the existence of a droplet in individual states after j time increments from the instant of its entry into the system is given by the relation

$$\mathbf{p}(j)^T = \mathbf{p}(0)^T \mathbf{P}^j, \quad (56)$$

where

$$\mathbf{p}(j) \equiv \{p(j)_i\}; \quad i = 1, \dots, N + 1 \quad (57)$$

is the column vector of the probability that the droplet exists in state i at the time j from its appearance in the system.

As has been mentioned the resulting probabilities of the appearance of a droplet in individual states in a given time instant of the process may be obtained by superposition of the probabilities valid for particles entering the system in individual time increments from the beginning of the process. In analogy to the simulation model we shall introduce the condition

C3: Starting from $t = 0$, q_0 identical droplets enter the system during each time increment. For the resulting vector of probabilities we then have

$$\begin{aligned} \mathbf{p}_n^T &= \sum_j \mathbf{p}(j); \quad j = 0, 1, \dots, n, \\ &= \mathbf{p}(0)^T \sum_j \mathbf{P}^j, \end{aligned} \quad (58)$$

The vector of distribution of the probability density in individual states is then

$$\mathbf{q}^T = \{q(j)_i\} = jq_0 \mathbf{p}(0)^T \sum_j \mathbf{P}^j; \quad j = 0, 1, \dots, n. \quad (59)$$

DISCUSSION

While assigning a definite numerical value to all remaining parameters of the simulation model and their combinations poses no problem the meaning of the sum $d + r + f$ calls for clarification. This sum represents the fractions of the whole content of a single stage transported during a single time increment Δt . Unlike the length increment Δl , whose value corresponds in case of a stagewise extractor to the height

of a construction stage, the time increment is adjustable. The ratio $f \Delta l / \Delta t$ though determines the rate of convective transport and its value is thus set by the conditions of the simulated process. Similarly, the value $(d + r) \Delta l / \Delta t$ determines the rate of axial mixing. From here we have that the sum $d + r + f$ is directly proportional to Δt . Clearly, the value of the sum should be taken sufficiently small in order to sufficiently closely represent the real continuous process by the discrete model.

If we deal with a differential contactor then also the length Δl is adjustable and the value of the sum $d + r + f$ will be indirectly proportional to the scale of velocity $\Delta l / \Delta t$. However, it must be considered that Δl appears also in the Peclet number (Eq. (33)) and its choice also affects the magnitude of \bar{r} .

The choice of the time increment affects also the magnitude of q_0 as may be apparent from the last of the relations (35). q_0 is thus proportional to $d + r + f$.

In view of what has been said above the choice of the time scale may affect also the properties of the random signal δd . With the decreasing time scale Δt the maximum amplitude of the signal diminishes and the characteristic frequency $\Delta l / \Delta t$ grows. This is true provided the changes of the random signal occur with the frequency $1 / \Delta t$. This limitation can be removed by introducing another parameter, τ , representing the ratio of the time increment of the generator of the random signal and the time scale

$$\tau = \Delta t_s / \Delta t. \quad (60)$$

The parameter τ thus affects the width of the band within which the autocorrelation function of the random signal δd has a nonzero value⁹.

As has been shown the simulation model expressed in terms of the expected values and the probability model are difference analogs of the differential model of van de Vusse. The advantage of the difference models rests in the ease of their solution both numerically and analytically as will be shown in the second part of this work. Another advantage of the difference models is that the time and spatial variation of the parameters can be more readily assessed. Moreover, if the real system is a stage-wise, the stagewise models allow their parameters to be assigned values associated with the physical nature of the process.

The stochastic simulation model, in addition, enables the random character of the true process to be expressed and the appropriate parameters d and τ represent suitable variables characterizing the source of random disturbance. It is apparent that the random character may exhibit not only axial mixing but also the other parameters such as *e.g.* the feed rates of the phases into the system *etc.* While fluctuation of these parameters can be in principle reduced by proper design and control elements the source of the scatter due to axial mixing is connected with the random nature of the flow within the system which cannot be effectively influenced by external means. At the same time the random character of the flow, beside the deterministic circula-

tion flows, is the source of the ultimate effect of axial mixing. In the calculations the random quantity $\delta_{i,j}$ is simulated by the generator of random numbers. The generator proposed here is one with a uniform distribution (15). Of course, other types of distribution may be chosen satisfying the model in order to examine the effect of the distribution of the random signal on the concentration distribution of the dispersion as a random response.

One of the advantages of the probabilistic model of the type of Markov's chain is that it enables the analytical solutions to be obtained easily (59) for the transient state. The theory of the Markov's systems permits also study of *e.g.* the rate of approach to the steady state by means of the properties of the transient matrix as will be shown in the second part of this work. As far as the relation between the stochastic and the probabilistic model presented above is concerned it is apparent that on averaging the fluctuation component in the first model (Eq. (17)–(23)) both models differ only formally in terminology and the Markov's model represents the averaged simulation model written in matrix notation. Let it be noted that both models enable easy generalization to more complex mechanisms of longitudinal mixing by *e.g.* removing the assumption *A3* and admitting transport over more than a single stage.

LIST OF SYMBOLS

d	fraction of droplets within a stage transported by random component of axial mixing
D	coefficient of axial dispersion L^2T^{-1}
$E_{(X)} = X$	expected (mean) value of variable X
f	fraction of droplets within a stage transported by convective flow
$H(c, h)$	uniform distribution with the mean c and half-width of interval h
i	sequence number of stage
j	sequence number of time increment
k	convective velocity in the second and the third section, LT^{-1}
Δl	length increment, height of stage, L
L	length of a column section, L
m	number of droplets in a stage
n	number of droplets in a unit volume, L^{-3}
N	sequence number of end section of column
p_{ik}	probability of droplet's transition from state i into k
$p(0)_i$	probability that a droplet enters initially state i
$p(j)_i$	probability that a droplet appears after j steps in state i
$\mathbf{p}(0)$	column vector of probabilities of initial states of droplets
$\mathbf{p}(j)$	column vector of probabilities of states of droplets after j steps
\mathbf{p}_n	column vector of state probabilities of droplets entering the process anytime from the onset
\mathbf{P}	transition matrix
q	density of flow of droplets at inlet, $L^{-2}T^{-1}$
q_0	number of droplets per unit area of column cross section entering during a single time increment, L^{-2}
$q(j)_i$	frequency of droplets in state i after j steps
\mathbf{q}	vector of frequencies of droplets in individual states after completion of the process

r	fraction of droplets in a single stage transported by nonrandom component of back flow
$\bar{r} = (d + r)/2f$	coefficient of backmixing
t	time, T
Δt	time increment of simulation model, T
Δt_s	time increment of generator of random signal, T
v	convective velocity in the first section, LT^{-1}
X	state of droplet
y	coordinate of length, L
Pe	Peclet number
δ	random variable defined by (12)
ν	dimensionless concentration of droplets defined by Eq. (28)
π	probability density of random variable
τ	dimensionless time increment of generator of random signal defined by Eq. (33)

Subscripts

i	sequence number of stage containing the examined particle
j	number of time steps
k	sequence number of stage entered by examined particle
1	first section of column
2	second section of column

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