# A STOCHASTIC MODEL OF A NONIDEAL MIXER. GENERAL APPROACH* 

V.Kudrna and H.Steidl<br>Department of Chemical Engineering, Institute of Chemical Technology, 16628 Prague 6

Received October 14th, 1974


#### Abstract

An attempt is made in the paper to describe the behaviour of a nonideal mixer using a model based on the concept of random motion of a mass point in a fluid the flow of which in an infinite unidimensional space is also generally random. Stochastic differential equations are used for the description on the assumption that the process is one of Markov. This procedure enables relations to be obtained for the transfer of a scalar quantity under the turbulent motion of the fluid.


The need for a more accurate description of the equipment of chemical technology as well as the growing size of such equipment has called for a change from the simple concept of an ideal mixer, or piston flow to a more complex concept of a nonideal mixer. In the latter, the properties of the batch change both in time and space. In view of the turbulent flow encountered often in such equipment the properties of the batch must be regarded as random functions of the above mentioned coordinates.

For description of a nonideal mixer the authors utilize various concepts regarding the stochastic character of the process within the equipment leading to the application of the theory of random functions: the stochastic operator ${ }^{1,2}$, random parameter functions ${ }^{3}$, continuous Markov's processes ${ }^{4}$, discontinuous Markov's processes ${ }^{5}$, stochastic differential equations ${ }^{6-8}$, or eventually their combination ${ }^{9-11}$.

This contribution is another attempt in this direction. It starts from the familiar concept of the diffusion motion of a particle ${ }^{12}$ modified by the random motion of the fluid surrounding the particle ${ }^{13,14}$. It is postulated that both processes may be regarded as diffusional Markov's processes ${ }^{15}$. Such processes may be described by stochastic differential equation ${ }^{16}$ and one can write down corresponding Kolmogorov's equations ${ }^{16,17}$ for the appropriate transitive probability densities.

From the Bernoulli formulation of the law of averages follows direct proportionality between the probability density for the event that the particle under consideration appears in a certain position on one hand and concentration of the dissolved component at the same position on the other hand. A similar conclusion pertains also to the

[^0]temperature so that the model enables description of any scalar quantity in a nonideal mixer under the random character of the flow. It will be shown that the decisive role in affecting the random character of the model behaviour of the scalar quantity plays the velocity of the flow of the fluid.

In order that we may avoid excessive complexity of the pertaining equations and clarify the chosen approach we shall confine ourselves to an infinite unidimensional space.

## THEORETICAL

## The Motion of the Tracer Particle in the Mixer

In accord with the just outlined approach we shall consider the following situation: A mixer as an infinite tube containing a flowing fluid (Fig. 1). The axis of cylindrical symmetry is identical with the axis $x$. The area of cross section, $S$, of the mixer is a constant, independent of $x$. The volume of the mixer confined between two cross sections at $x$ and $x+\Delta x$ is designated by $\Delta M$.


Fig. 1
Sketched Motion of Tracer Particle within the Mixer
$\longrightarrow$ Trajectory of center of gravity of the fluid volume $\Delta U, \ldots-\ldots$ trajectory of tracer particle.

At a time $t=0$ a tracer particle, $P$, is placed into the center of gravity of a volume of the fluid, $\Delta U$. The motion of the tracer particle in the fluid is detectable and its mass, $m_{p}$, is negligible with respect to the mass of the volume $\Delta U$. The characteristic linear dimension of this volume is negligible with respect to the diameter of the mixer.

As we consider only the unidimensional problem the motion of the particle and the center of gravity of the volume $\Delta U$ will be determined solely by the axial coordinate, i.e. perpendicular projection onto the axis $x$. The instantaneous position of the particle, $X_{\mathrm{p}}(t)$ is then the superimposed position, $X_{\mathbf{k}}(t)$, of the center of gravity of the fluid volume $\Delta U$, onto the relative distance of the particle, $X_{\mathrm{r}}(t)$, from the center of gravity of $\Delta U$.

$$
\begin{equation*}
X_{\mathrm{p}}(t)=X_{\mathrm{k}}(t)+X_{\mathrm{r}}(t) \tag{1}
\end{equation*}
$$

The velocity, $V_{k}(t)$, of the center of gravity of $\Delta U$ is defined by

$$
\begin{equation*}
V_{\mathrm{k}}(t)=\mathrm{d} X_{\mathrm{k}}(t) / \mathrm{d} t . \tag{2}
\end{equation*}
$$

All quantities just written may be generally random functions of time.
Now it is possible to specify the set of simplifying assumptions enabling a quantitative expression of the particle's motion:

1) The nonrandom forces acting on $\Delta U$ are such that the resulting force is generally a function of position and velocity of its center of gravity and (explicitely) of time.

Note: These forces are nonrandom in the sense that they are deterministic functions of their arguments.
2) The volume $\Delta U$ is subject to the action of a random force characterized by impulse equaling the product of the (deterministic) function of generally position and velocity of its center of gravity and (explicitely) time times the Wiener's process ${ }^{18}$, $W_{k}(t)$.
3) The interaction between the tracer particle and the molecules of the fluid are random and such that the relative position of the particle with respect to the center of gravity of the volume $\Delta U$ is proportional to the Wiener's process, $W_{\mathrm{r}}(t)$. The latter process is then independent of the former. The coefficient of proportionality is a constant.
4) The velocity of the fluid at the position of the particle does not significantly differ from the velocity of the center of gravity of the volume $\Delta U$.

Note: This assumption poses, as will be shown in the discussion, certain limitations on the quantities in the preceding assumptions.
5) The residence time of the tracer particle within the mixer is generally a random variable depending neither on particle's position nor time required for the particle to reach this position.

With regard to the assumptions 1 ) and 2 ) one can now write down the equation of motion of the center of gravity of the volume $\Delta U$ as a stochastic differential equation ${ }^{18-20}$

$$
\begin{equation*}
\mathrm{d} V_{\mathbf{k}}=g\left(X_{\mathrm{k}}, V_{\mathbf{k}}, t\right) \mathrm{d} t+h\left(X_{\mathbf{k}}, V_{\mathbf{k}}, t\right) \mathrm{d} W_{\mathrm{k}} . \tag{3}
\end{equation*}
$$

The function $g($.$) represents the intensity of the nonrandom force determined by the$ assumption 1 ). The function $h($.$) and the Wiener's process W_{\mathrm{k}}(t)$ characterize the random force specified in assumption 2).

According to the assumption 3) the following stochastic differential equation describing the relative motion of the particle is also valid.

$$
\begin{equation*}
\mathrm{d} X_{\mathrm{r}}=\sigma_{\mathrm{r}} \mathrm{~d} W_{\mathrm{r}} \quad[t<T] \tag{4}
\end{equation*}
$$

where $\sigma_{\mathrm{r}}$ is a proportionality constant. The condition in the bracket expresses the fact that Eq. (4) holds with respect to assumption 5) only up to a (random) time instant $T$ when the particle disappears.
With certain requirements put on the functions $g($.$) and h($.$) regarding their con-$ tinuity and boundeness it can be shown that the functions $V_{\mathrm{k}}(t)$ and $X_{\mathrm{k}}(t)$ in Eqs (2) and (3) constitute a two dimensional Markov's diffusion process with the corresponding Kolmogorov's forward equation as ${ }^{21,22}$

$$
\begin{equation*}
\frac{\partial f_{\mathrm{k}}^{\prime}}{\partial t}+v \frac{\partial f_{\mathrm{k}}^{\prime}}{\partial x}+\frac{\partial}{\partial v}\left[g(x, v, t) f_{\mathrm{k}}^{\prime}\right]-\frac{1}{2} \frac{\partial^{2}}{\partial v^{2}}\left[h^{2}(x, v, t) f_{\mathrm{k}}^{\prime}\right]=0 . \tag{5}
\end{equation*}
$$

The transitive probability density, $f_{\mathbf{k}}^{\prime}($.$) , is defined by$

$$
\begin{align*}
& f_{\mathrm{k}}^{\prime}\left(x, v ; t \mid x^{0}, v^{0}\right) \equiv \lim _{\substack{\Delta x \rightarrow 0 \\
\Delta v \rightarrow 0}} \frac{1}{\Delta x \Delta v} . \\
& \quad . P\left\{x \leqq X_{\mathrm{k}}(t)<x+\Delta x ; v \leqq V_{\mathrm{k}}(t)<v+\Delta v \mid X_{\mathrm{k}}(0)=x^{0} ; V_{\mathrm{k}}(0)=v^{0}\right\} . \tag{5a}
\end{align*}
$$

With respect to the fact that the mixer is infinite it suffices to consider only the initial condition for Eq. (5). The position and velocity of the center of gravity of the volume $\Delta U$ at the time $t=0$ may be generally random; the initial probability density, $f_{\mathrm{k}}^{0}\left(x^{0}, v^{0}\right)$, must be specified. A solution of Eq. (5) is

$$
\begin{equation*}
f_{k}(x, v ; t)=\iint_{-\infty}^{+\infty} f_{\mathbf{k}}^{\prime}\left(x, v ; t \mid x^{0}, v^{0}\right) f_{\mathbf{k}}^{0}\left(x^{0}, v^{0}\right) \mathrm{d} x^{0} \mathrm{~d} v^{0} \tag{6}
\end{equation*}
$$

The Kolmogorov's equation corresponding to Eq. (4) is written first for the case that the tracer particle does not disappear within a finite time interval, i.e. when $T \rightarrow \infty$. Then we have

$$
\begin{equation*}
\frac{\partial f_{\mathrm{r}}^{\prime}}{\partial t}-\frac{1}{2} \sigma_{\mathrm{r}}^{2} \frac{\partial^{2} f_{\mathrm{r}}^{\prime}}{\partial x_{\mathrm{r}}^{2}}=0 \tag{7}
\end{equation*}
$$

where

$$
\begin{equation*}
f_{\mathrm{r}}^{\prime}\left(x_{\mathrm{r}} ; t \mid x_{\mathrm{r}}^{0}\right) \equiv \lim _{\Delta x_{\mathrm{r}} \rightarrow 0} \frac{1}{\Delta x_{\mathrm{r}}} P\left\{x_{\mathrm{r}} \leqq X_{\mathrm{r}}(t)<x_{\mathrm{r}}+\Delta x_{\mathrm{r}} \mid X_{\mathrm{r}}(0)=x_{\mathrm{r}}^{0}\right\} \tag{7a}
\end{equation*}
$$

is the transitive probability density enabling the distribution of the distance of the tracer particle from the center of gravity of $\Delta U$ to be determined.

If at $t=0$ this position is identical with that of the center of gravity, the initial condition is the Dirac function $\delta\left(x_{\mathrm{r}}^{0}\right)$ and the solution is

$$
\begin{equation*}
f_{\mathrm{r}}\left(x_{\mathrm{r}} ; t\right)=\int_{-\infty}^{+\infty} f_{\mathrm{r}}^{\prime}\left(x_{\mathrm{r}} ; t \mid x_{\mathrm{r}}^{0}\right) \delta\left(x_{\mathrm{r}}^{0}\right) \mathrm{d} x_{\mathrm{r}}^{0}=f_{\mathrm{r}}^{\prime}\left(x_{\mathrm{r}} ; t \mid 0\right) . \tag{8}
\end{equation*}
$$

In case that $T$ takes finite values one can write first with respect to assumption 5) a relation for the distribution function for the time of existence of the tracer particle $T$ within the mixer ${ }^{23}$

$$
\begin{equation*}
\mathrm{d} F_{\mathrm{t}} / \mathrm{d} t=-\lambda F_{\mathrm{t}} \tag{9}
\end{equation*}
$$

where $F_{1}(t) \equiv P\{t<T\}$ and $\lambda$ is a constant indirectly proportional to the time of existence of the particle. The initial condition is clearly $F_{\mathrm{t}}(0)=1$. The function $F_{\mathrm{t}}(t)$ according to the assumption 5) is independent of particle's position and hence of the probability density given by Eq.(8). The probability density of the function $X_{r}(t)$ written in Eq. (4) is thus generally given by the expression

$$
\begin{equation*}
f_{\mathrm{rI}}\left(x_{\mathrm{r}} ; t\right)=f_{\mathrm{r}}\left(x_{\mathrm{r}} ; t\right) \cdot F_{\mathrm{l}}(t) . \tag{10}
\end{equation*}
$$

Eqs (7) and (10) indicate that the analytical form of this function can be easily found:

$$
f_{\mathrm{r}}\left(x_{\mathrm{r}} ; t\right)=\left(2 \pi \sigma_{\mathrm{r}}^{2} t\right)^{-1 / 2} \cdot \exp \left[-\left(x_{\mathrm{r}}^{2} / 2 \sigma_{\mathrm{r}}^{2} t\right)-\lambda t\right] .
$$

Finally, one can write the relation characterizing the distribution of the random function $X_{\mathrm{p}}(t)$, i.e. position of the tracer particle with respect to the mixer. As the processes $W_{\mathrm{k}}(t)$ and $W_{\mathrm{r}}(t)$, according to the assumption 3) are mutually independent, the processes $X_{\mathrm{r}}(t)$ and $X_{\mathrm{k}}(t)$ are also independent as follows from Eq. (2) and (4). With respect to Eq. (1) the convolution integral can be written as:

$$
\begin{equation*}
f_{\mathrm{pk}}(x, v ; t)=\int_{-\infty}^{+\infty} f_{\mathrm{k}}\left(x-x_{\mathrm{r}}, v ; t\right) f_{\mathrm{r}}\left(x_{\mathrm{r}} ; t\right) \mathrm{d} x_{\mathrm{r}} \tag{1I}
\end{equation*}
$$

It is apparent that the function $f_{\mathrm{pk}}($.$) is a two-dimensional probability density$ determining simultaneously the distribution of particle's position, $X_{\mathrm{p}}(t)$, in the mixer and the velocity, $V_{k}(t)$, of the center of gravity of the fluid, $\Delta U$, while, according to the assumption 4) this quantity can be approximately regarded as the fluid velocity at the point of the tracer particle.

In order that we may obtain the unidimensional probability density for the random function $X_{p}(t)$ the conditional probability density at time $t$ is written as

$$
\begin{equation*}
f_{\mathrm{p}}(x \mid v ; t)=f_{\mathrm{pk}}(x, v ; t) / f_{\mathrm{v}}(v ; t) \tag{12}
\end{equation*}
$$

where $f_{\mathrm{v}}($.$) is the marginal probability density for the velocity V_{\mathbf{k}}(t)$. This may be found by integration of the function $f_{k}($.$) , given by Eq. ( \sigma$ ), over the whole mixer

$$
\begin{equation*}
f_{v}(v ; t)=\int_{-\infty}^{+\infty} f_{k}(x, v ; t) \mathrm{d} x . \tag{13}
\end{equation*}
$$

The function $f_{p}($.$) thus indicates the probability of the event that the particle still$ exists at the time $t$ elapsed from the beginning of observation within the volume of the mixer $\Delta M$ (the thickness $\Delta x$ of which approaches to zero) provided that the velocity of the center of gravity at the same time instant (and approximately also the velocity of the volume $\Delta M$ ) takes the value of $v$ :

$$
\begin{equation*}
f_{\mathrm{p}}(x \mid v ; t) \equiv \lim _{\Delta x \rightarrow 0} \frac{1}{\Delta x} P\left\{x \leqq X_{\mathrm{p}}(t)<x+\Delta x \mid V_{\mathrm{k}}(t)=v ; t<T\right\} \tag{14}
\end{equation*}
$$

The quantity $v$ may thus be regarded as a parameter of the above distribution at an instant $t$.

The Relation between the Probability Density for the Particle's Position and Concentration or Temperature within the Mixer

It will be shown now that there exists a simple correlation between the function $f_{\mathrm{p}}($. and scalar quantities (temperature or concentration) usually used for description of some of the phenomena within the mixer:

Consider a set of $N$ particles of equal mass the motion of which obeys the relations given in the preceding paragraph. According to a particular form of the law of averages - the Bernoulli law - one can write ${ }^{24}$ for each $\varepsilon>0$ that

$$
\begin{equation*}
\lim _{N \rightarrow \infty} P\left\{\mid \sum_{i=1}^{N} I_{\mathrm{i}} / N-P\left\{x \leqq X_{\mathrm{p}}(t)<x+\Delta x \mid V_{\mathrm{k}}(t)=v ; t<T\right\} \geqq \geqq\right\}=0 \tag{15}
\end{equation*}
$$

$I_{i}$ is an indicator ${ }^{25}$ of the random event that at a time $T$ the i-th particle fulfils the condition within the inner curly brackets. The sum in the numerator thus designates the number of particles appearing at a time $t$ within the volume of the mixer $\Delta M$ at an instantaneous fluid velocity equal $v$.

For a large set of particles we thus have an approximate equation following from Eq. (15) taking into account also Eq. (14):

$$
n \equiv \sum_{i=1}^{N} I_{i} \approx N \int_{x}^{x+\Delta x} f_{\mathrm{p}}(y \mid v ; t) \mathrm{d} y
$$

Multiplying this relation by the mass of the particles, $m_{\mathrm{p}}$, and dividing it by the volume of the mixer we arrive at the relation between the concentration of the particles, $c($.$) , and the probability density defined in Eq. (14)$

$$
c(x, v, t)=\lim _{\Delta M \rightarrow 0} m_{\mathrm{p}} n / \Delta M=\left(N m_{\mathrm{p}} / S\right) \lim _{\Delta x \rightarrow 0}(1 / \Delta x) \int_{x}^{x+\Delta x} f_{\mathrm{p}}(y \mid v ; t) \mathrm{d} y .
$$

From this we have that

$$
\begin{equation*}
c(x, v, t)=(m / S) f_{\mathrm{p}}(x \mid v ; t), \tag{16a}
\end{equation*}
$$

which is valid for large $N$ with sufficient accuracy. The symbol $m$ designates the mass of all particles which appeared at the instant $t=0$ within the mixer.
If it is assumed that the energy transfer within the fluid obeys an analogous mechanism as the one just described a similar equation for the temperature distribution of the fluid, $\Theta($.$) , is$

$$
\begin{equation*}
\Theta(x, v, t)=\left(\Delta H / S \varrho c_{\mathrm{p}}\right) f_{\mathrm{p}}(x \mid v ; t), \tag{16b}
\end{equation*}
$$

where $\varrho$ and $c_{\mathrm{p}}$ designate respectively density and heat capacity of the fluid. $\Delta H$ is the total enthalpy of the fluid at the time $t=0$.

Let us denote now a general scalar quantity by the symbol $q($.$) and write down$ Eqs (16a), (16b) in a single expression

$$
\begin{equation*}
q(x, v, t)=k f_{\mathrm{p}}(x \mid v ; t) . \tag{16}
\end{equation*}
$$

The particular form and dimension of the proportionality constant $k$ depends clearly on the type of the scalar quantity.

## The Effect of the Velocity of Fluid Flow on the Scalar Quantity

It will be shown below that the scalar quantity just defined is, according to the underlying model concept, significantly affected by the character of the fluid flow.
Consider a fixed time instant $t$. From Eq. (16) and (12) it follows that the scalar quantity $q(x, v, t)$ at the time $t$ is a function of the parameter $v$ the distribution of which at the same instant is described by the probability density $f_{v}(v, t)$ given in Eq. (13). The scalar quantity $q($.$) may thus be though of as a function of the random$ variable $V_{\mathrm{k}}$ at the given instant ${ }^{26} t$.
The distribution of this random variable, however, is defined (see Eqs (12) and (13)) for the same region as the scalar quantity $q($.$) itself. Thus for all instants t \geqq 0$ one can write down formally the scalar quantity $q($.$) as a nonrandom function of the ran-$ dom function of time, $V_{\mathbf{k}}(t): q\left(x, V_{\mathbf{k}}(t), t\right)$.

The scalar quantity - concentration or temperature - is thus written as a random function of time (and position) only if the velocity of the fluid flow is a random function of time:

$$
\begin{equation*}
Q(x, t)=q(x, V(t), t) \tag{17}
\end{equation*}
$$

The symbol $Q($.$) designates a scalar quantity as a random function of the above vari-$ ables.

This consideration enables the distribution function, or the probability density of the scalar quantity $Q($.$) to be found because for each t$ one can write ${ }^{27}$

$$
\begin{gather*}
f_{q}(p ; x, t) \equiv \lim _{\Delta p \rightarrow 0} \frac{1}{\Delta p} P\{p \leqq Q(x, t)<p+\Delta p= \\
=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} \exp (-i \omega p) \mathrm{d} \omega \int_{-\infty}^{+\infty} \exp [i \omega q(x, v, t)] f_{v}(v ; t) \mathrm{d} v \tag{18}
\end{gather*}
$$

where $\omega$ is the variable of the Fourier transform.
One can also find easily the expected value of the scalar quantity $Q($.

$$
\begin{equation*}
E[Q(x, t)]=E\left[q\left(x, V_{\mathrm{k}}(t), t\right)\right]=\int_{-\infty}^{+\infty} q(x, v, t) f_{\mathrm{v}}(v ; t) \mathrm{d} v \tag{19}
\end{equation*}
$$

and its variance

$$
\begin{align*}
& \operatorname{Var}[Q(x, t)] \equiv E\left[q^{2}\left(x, V_{\mathrm{k}}(t), t\right)\right]-E^{2}\left[q\left(x, V_{\mathrm{k}}(t), t\right)\right]= \\
& =\int_{-\infty}^{+\infty} q^{2}(x, v, t) f_{\mathrm{v}}(v ; t) \mathrm{d} v-\left[\int_{-\infty}^{+\infty} q(x, v, t) f_{\mathrm{v}}(v ; t) \mathrm{d} v\right]^{2} . \tag{20}
\end{align*}
$$

For the calculation of the correlation and the autocorrelation function of the scalar quantity $Q($.$) one needs the compound probability density for the velocity of the fluid$ at two time instants $t$ and $\tau$ :

$$
\begin{gathered}
f_{v v^{\prime}}\left(v, v^{\prime} ; t, \tau\right)=\lim _{\substack{\Delta v \rightarrow 0 \\
\Delta v^{\prime} \rightarrow 0}} \frac{1}{\Delta v \Delta v^{\prime}} P\left\{v \leqq V_{\mathrm{k}}(t)<v+\Delta v \mid V_{\mathrm{k}}(\tau)=v^{\prime}\right\} \\
. P\left\{v^{\prime} \leqq V_{\mathrm{k}}(\tau)<v^{\prime}+\Delta v^{\prime}\right\} \quad[0<\tau<t]
\end{gathered}
$$

This function can be found by considering the definition of the transitive probability defined in Eq. ( $5 a$ ) for the time instants $t$ and $\tau$ and the probability density determined
by Eq. (6) for the time instant $\tau$ as a double marginal distribution:

$$
\begin{equation*}
f_{\mathrm{v}}\left(v, v^{\prime} ; t, \tau\right)=\iint_{-\infty}^{+\infty} f_{\mathbf{k}}^{\prime}\left(x, v ; t \mid x^{\prime}, v^{\prime} ; \tau\right) f_{\mathrm{k}}\left(x^{\prime}, v^{\prime} ; \tau\right) \mathrm{d} x \mathrm{~d} x^{\prime} \tag{21}
\end{equation*}
$$

The relation for the correlation function of the scalar quantity $Q($.$) then follows$ from the equation

$$
\begin{gathered}
\operatorname{Cov}\left[Q(x, t) \cdot Q\left(x^{\prime}, \tau\right)\right] \equiv E\left[q\left(x, V_{\mathrm{k}}(t), t\right) \cdot q\left(x^{\prime}, V_{\mathrm{k}}(\tau), \tau\right)\right]- \\
-E\left[q\left(x, V_{\mathbf{k}}(t), t\right)\right] \cdot E\left[q\left(x^{\prime}, V_{\mathrm{k}}(\tau), \tau\right)\right],
\end{gathered}
$$

where the symbols $q\left(x, V_{\mathbf{k}}(t), t\right)$ and $q\left(x^{\prime}, V_{\mathrm{k}}(\tau), \tau\right)$ designate the effect of the velocity of the fluid flow on the scalar quantity at the time $t$ or $\tau$. With the aid of Eqs (19) and (21) we thus finally have

$$
\begin{gather*}
\operatorname{Cov}\left[Q(x, t) \cdot Q\left(x^{\prime}, t\right)\right]=\iint_{-\infty}^{+\infty} q(x, v, t) q\left(x^{\prime}, v^{\prime}, \tau\right) f_{\mathrm{vv}}\left(v, v^{\prime} ; t, \tau\right) \mathrm{d} v \mathrm{~d} v^{\prime}- \\
-\int_{-\infty}^{+\infty} q(x, v, t) f_{v}(x, t) \mathrm{d} v \cdot \int_{-\infty}^{+\infty} q\left(x^{\prime}, v^{\prime}, t\right) f_{\mathrm{v}}\left(v^{\prime}, \tau\right) \mathrm{d} v^{\prime} \tag{22}
\end{gather*}
$$

Putting $x=x^{\prime}$ in the last equation one obtains an expression for the autocorrelation function of the scalar quantity $Q($.$) .$

In the outlined manner one could find also multiple probability densities and eventually higher moments of the scalar quantity $Q($.$) .$

## Diffusion* Equation for a Scalar Quantity

On the basis of the model concept developed in the preceding paragraphs it is possible to write down formally a differential equation permitting application of these concepts to the description of the transport processes involving scalar quantities: From Eqs (6) through (10) one obtains first by simple algebraic operations the relation

$$
\frac{\partial f_{\mathrm{kt}}}{\partial t}+v \frac{\partial f_{\mathrm{kt}}}{\partial x}+\lambda f_{\mathrm{kt}}-\frac{1}{2} \sigma_{\mathrm{r}}^{2} \frac{\partial^{2} f_{\mathrm{kt}}}{\partial x_{\mathrm{r}}^{2}}+\frac{\partial}{\partial v}\left(g f_{\mathrm{kt}}\right)-\frac{1}{2} \frac{\partial^{2}}{\partial v^{2}}\left(h^{2} f_{\mathrm{kt}}\right)=0
$$

where $f_{\mathrm{kt}}=f_{\mathrm{k}}(x, v ; t) . f_{\mathrm{rt}}\left(x_{\mathrm{r}} ; t\right)$. Next we exchange the sequence of the variables and carry out integration shown in Eq. (11). Provided that $f_{\mathrm{k}}\left(x-x_{\mathrm{r}}, v ; t\right) \cdot f_{\mathrm{rt}}\left(x_{\mathrm{r}} ; t\right)$

* The term "diffusion" is used in the usual sense of Markov's processes ${ }^{28}$.
converges to zero with $x_{\mathrm{r}}$ growing to infinity and with respect to Eqs (14) and (16) we obtain the following differential equation:

$$
\begin{gather*}
\frac{\partial}{\partial t}\left(q \cdot f_{v}\right)+v \frac{\partial}{\partial x}\left(q \cdot f_{v}\right)+\lambda\left(q \cdot f_{v}\right)-\frac{1}{2} \sigma_{\mathrm{r}}^{2} \frac{\partial^{2}}{\partial x^{2}}\left(q \cdot f_{v}\right)+ \\
+\frac{\partial}{\partial v}\left(g^{*} \cdot q \cdot f_{v}\right)-\frac{1}{2} \frac{\partial^{2}}{\partial v^{2}}\left(h^{2 *} \cdot q \cdot f_{v}\right)=0 . \tag{23}
\end{gather*}
$$

The function $g^{*}($.$\left.) (and similarly also h^{2 *}().\right)$ is defined by
$g^{*}(x, v, t) \equiv\left\{\begin{array}{r}\left\{\begin{array}{l}\left\{\int_{-\infty}^{+\infty} g\left(x-x_{r}, v, t\right) f_{\mathrm{k}}\left(x-x_{\mathrm{r}}, v ; t\right) f_{\mathrm{r}}\left(x_{\mathrm{r}} ; t\right) \mathrm{d} x_{\mathrm{r}}\right.\end{array}\right\}\left(f_{\mathrm{pk}}(x, v ; t)\left[f_{\mathrm{pk}}(.)>0\right]\right. \\ \square \quad\left[f_{\mathrm{pk}}(.)=0\right]\end{array}\right.$
Eq. (23) permits each of its terms to be assigned a simple physical meaning. With the same aim it can be integrated over the whole region of the variable $v$ and with respect to Eq. (19) to obtain

$$
\begin{gather*}
\frac{\partial}{\partial t} E[Q(x, t)]+\frac{\partial}{\partial x} \operatorname{Cov}[Q(x, t) V(t)]+E[V(t)] \frac{\partial}{\partial x} E[Q(x, t)]+\lambda E[Q(x, t)]- \\
-\frac{1}{2} \sigma_{\mathrm{r}}^{2} \frac{\partial^{2}}{\partial x^{2}} E[Q(x, t)]=0 \tag{24}
\end{gather*}
$$

where

$$
\begin{gathered}
\operatorname{Cov}[Q(x, t) v(t)]=\int_{-\infty}^{+\infty} v q(x, v, t) f_{v}(v ; t) \mathrm{d} v-\int_{-\infty}^{+\infty} q(x, v, t) f_{v}(v ; t) \mathrm{d} v . \\
\cdot \int_{-\infty}^{+\infty} v f_{v}(v ; t) \mathrm{d} v .
\end{gathered}
$$

The last two terms of Eq. (23) vanish after integration if we adopt the assumption that the functions $f v($.$) and \partial / \partial v f_{v}($.$) vanish with the variable growing to infinity.$

## DISCUSSION

The model concept described above and the relations following from it enable the transport of a scalar quantity - temperature or concentration - to be described in the situation under consideration, i.e. in a one-dimensional space. This fact stands out clearly mainly from Eq. (23) which can be compared with the usually used trans-
port equations. The expression $q . f_{v}$ may be interpreted as the product of the scalar quantity $q(x, v, t)$ and the coefficient $f_{\mathrm{v}}(v, t)$ characterizing the "behaviour" of the parameter $v$. The latter, as has been shown, characterizes the effect of the velocity of fluid flow on the scalar quantity.

The first term in Eq. (23), characterizing the unsteadiness of the process, may be regarded as an accumulation term of the scalar quantity. The third term of the same equation expresses generally the loss of the scalar quantity either due to a first order chemical reaction, in case that $q($.$) stands for concentration, or the loss of heat in case$ of temperature. The fourth term is the usual expression for molecular diffusion. The second term of Eq. (23) may be regarded as the expression of the convective transfer. Formally it symbolizes the relation between the velocity of the fluid flow and the scalar quantity. It is apparent that had this term not been present, Eq. (23) could be separated into two mutually independent relations for $q($.$) and f_{v}($.$) .$

The fifth and the sixth term of the equation describe quantitatively the fluid velocity: As it is indicated by assumptions 1) -4) and the relations following from these, the fifth term expresses the effect of nonrandom forces and the sixth term that of random forces acting on the fluid. The last but one term may thus be thought of as the source of convective (nonrandom) flow and the last one as the source of random, i.e. turbulent, velocity fluctuations.

Eq. (24) following from Eq. (23) is then the usually used expression for description of the transport of a scalar quantity under a unidimensional turbulent flow of the fluid ${ }^{13}$.

Eq. (23) thus permits description of the simultaneous effect of all means of transport usually taken into account: molecular, turbulent and convective plus the expression for the source term of the scalar quantity. The latter, of course, could not be expressed in the general form owing to the character of the model concept.

Also the assumption enabling the exchange of the velocity of the center of gravity of the fluid volume $\Delta U$ by the fluid velocity at the tracer particle is generally valid only if the forces acting on the center of gravity (see assumption 1) and 2) are explicit functions of position $X_{k}(t)$ and hence that the fluid velocity is not a function of the coordinate of position. In the opposite case this assumption can be adopted only if the random motion of the particle according to the assumption 3) is negligible with respect to the random motion of the fluid volume $\Delta U$. In view of the consideration in the preceding paragraphs this means that molecular transport of the scalar quantity in each instant must be negligible with respect to the turbulent transport.

The presented model concept thus enables, despite of the just described limitations, the effect of the hydrodynamics of the fluid flow to be described on the transfer of a scalar quantity. For description of a definite situation the functions $g($.$) and h($. in Eq.(3) or derived equations must be, of course, known. This can be accomplished for instance on the basis of additional concrete physical concepts regarding the fluid flow within the equipment in question.

In principle, the estimates of these functions describing the motion of the center of gravity of the volume $\Delta U$ can be found experimentally with the aid of a suitable tracer particle ${ }^{29}$. This particle must follow with sufficient accuracy the motion of this volume of the fluid.

## LIST OP SYMBOLS

| $c$ | volume concentration ( $\mathrm{kg} \mathrm{m}^{3-}$ ) |
| :---: | :---: |
| $c_{p}$ | specific heat of fluid ( $\mathrm{Jkg}^{-1} \mathrm{~K}^{-1}$ ) |
| $F$ | distribution function |
| $f$ | probability density |
| $g$ | intensity of nonrandom force ( $\mathrm{ms}^{-2}$ ) |
| H | enthalpy (J) |
| $h$ | function characterizing random force ( $\mathrm{ms}^{-3 / 2}$ ) |
| $I$ | indicator |
| $k$ | proportionality constant |
| $\Delta M$ | part of mixer's volume ( $\mathrm{m}^{3}$ ) |
| $m$ | mass (kg) |
| $N$ | total number of tracer particles |
| $n$ | number of tracer particles in volume $\Delta M$ |
| $P$ | tracer particle |
| $p$ | scalar parameter |
| $Q$ | scalar quantity (random function) |
| $q$ | scalar quantity |
| $S$ | area of cross section of mixer ( $\mathrm{m}^{2}$ ) |
| $T$ | residence time of tracer particle (s) |
| $t$ | time (s) |
| $\Delta U$ | small volume of fluid ( $\mathrm{m}^{3}$ ) |
| $V$ | velocity (random function) (m s ${ }^{-1}$ ) |
| $v$ | velccity ( $\mathrm{m} \mathrm{s}^{-1}$ ) |
| W | Wiener's process (random function) ( $\mathrm{s}^{1 / 2}$ ) |

$X \quad$ coordinate of position (random function) (m) coordinate of position (m)
$\varepsilon \quad$ positive number
$\lambda$ inverse mean residence time of tracer particle ( $\mathrm{s}^{-1}$ )
$\varrho \quad$ fluid density $\left(\mathrm{kg} \mathrm{m}^{-3}\right)$
$\sigma_{r} \quad$ characteristic of relative motion of tracer particle ( $\mathrm{m} \mathrm{s}^{-1 / 2}$ )
$\Theta \quad$ temperature (K)
$\tau \quad$ time ( s )
$\omega \quad$ Fourier transform parameter
$N$ total number of tracer particles
$n \quad$ number of tracer particles in volume
Subscripts
$i$ element of sequence
$k$ fluid
$p$ particle
$q \quad$ scalar quantity
$r$ relative position of tracer particle
$t$ residence time of tracer particle

## Superscripts

0 initial
, transitive

## REFERENCES

1. Václavek V.: This Journal 32, 3646 (1967).
2. Václavek V.: Chem. Eng. Sci. 22, 1209 (1967).
3. Katz S.: Chem. Eng. Sci. 9, 61 (1958).
4. Steidl H.: This Journal 25, 515 (1960).
5. Gibilaro L. G., Kropholler H. W., Spikins D. J.: Chem. Eng. Sci. 22, 517 (1967).
6. King R. P.: Chem. Eng. Sci, 23, 1035 (1968).
7. King R. P.: Ind, Eng. Chem. Fundam. 9., 190 (1970).
8. King R. P.: Chem. Eng. Sci. 26, 729 (1971).
9. Krambeck F. J., Shinnar R., Katz S.: Ind. Eng. Chem. Fundam. 6, 276 (1967).
10. Krambeck F. J., Shinnar R., Katz S.: Can. J. Chem. Eng. 45, 203 (1967).
11. Krambeck F. J., Katz S., Shinnar R.: Ind. Eng. Chem. Fundam. 8, 431 (1969).
12. Ito K., McKean H. P.: Diffusion Processes and their Sample Paths. Springer, Berlin 1965.
13. Hinze J. V.: Turbulence. An Introduction to Its Mechanism and Theory. McGraw-Hill. New York 1959.
14. Soo S. L.: Fluid Dynamics of Multiphase Systems, p. 46. Moscow 1971.
15. Dynkin E. B.: Markovskiie Processy. Fizmatgiz, Moscow 1963.
16. Gikhman J. J., Skorokhod A. V.: Stokhasticheskiie Differentsialnye Uravnenia. Naukova dumka, Kicev 1968.
17. Sveshnikov A. A.: Prikladnye Metody teorii Sluchajnykh funktsii. Nauka, Moscow 1968.
18. See ref. 16, p. 8.
19. See ref. 16, p. 33 and 275.
20. See ref. 16, p. 62 and 290.
21. See ref. 16, p. 1012 and 299.
22. See ref. 17, p. 285.
23. Feller W.: An Introduction to Probability Theory and its Applications, p. 8. Wiley, New York 1966.
24. Loéve M.: Probability Theory, p. 22, Izd. Inostr. Lit., Moscow 1962 (in Russian).
25. See ref. 24, p. 17.
26. Fisz M.: Wahrscheinlichkeitsrechnung und Mathematische Statistik, p. 148. Deutscher Verlag der Wissenschaften, Berlin 1958.
27. Pugachev V. S.: Teoria Sluchainykh Funkrii i ee Primeneniia $k$ Zadacham Avtomaticheskogo Upravlenia, p. 136, Gosizdat Tekh. Teor. Lit., Moscow 1957.
28. See ref. 16, p. 62.
29. Steidl H.: Chem. Listy 52, 839 (1958).

Translated by V. Stanĕk.


[^0]:    * Part XLIII in the series Studies on Mixing; Part XLII: This Journal 40, 3443 (1975).

