

## A STOCHASTIC MODEL OF A NONIDEAL MIXER. CONCENTRATION TRANSIENTS IN A BATCH SYSTEM\*

V. KUDRNA and J. VLČEK

*Department of Chemical Engineering,  
Institute of Chemical Technology, 166 28 Prague 6*

Received October 14th, 1974

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A model concept is proposed in the paper enabling description of concentration transients of a dissolved tracer solute in a nonideally mixed liquid batch assuming a random motion of the liquid. The model concept satisfactorily agrees with the experimental data.

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A general model has been proposed in the preceding communication<sup>1</sup> for description of one dimensional transport of a scalar quantity in a nonideal mixer. Using the concept of mutual motion of a tracer particle and fluid in the mixer the appropriate stochastic differential equations were written down. These equations yielded the diffusion equation describing the transport of concentration or temperature of the fluid. The application of this concept to be presented here enables the transient development of concentration of a tracer solute (*e.g.* solution of an electrolyte) to be described. The tracer solute is added at the onset of the process to the mechanically mixed batch.

### THEORETICAL

Let us assume that the process under consideration, *i.e.* the change of concentration of the tracer solute, will be observed in the following set-up: An impeller is located (Fig. 1) in a cylindrical vessel and induces axially symmetric flow of the batch with respect to the axis of symmetry of the vessel. The flow is random and stationary. At a time instant  $t = 0$  a certain volume of the tracer solution is injected at a point  $x_0$  on the level of the mixed batch. The volume of the tracer solution is negligible with respect to the total volume of the batch and the duration of injection is negligible with respect to the time of homogenation of the tracer solution in the batch.

The tracer solution is carried by the fluid and first enters the rotor region of the impeller to be dispersed uniformly over the horizontal plane. Next, it follows a circulatory motion shown schematically in Fig. 1. By this process the tracer solution is being dispersed more and more uniformly into the whole volume of the batch.

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\* Part XLIV in the series: Studies on Mixing; Part XLIII: This Journal 40, 3781 (1975).

The presence of the tracer solution is indicated by a detector located in the radial stream of the fluid emerging from the rotor region of the impeller.

Let us suppose that the dimensions of the detector are negligible with respect to the size of the equipment and hence may be regarded as a point in the volume of the batch. The circulatory motion of the elements of the tracer particle projected onto a straight line drawn through the point of the detector parallel to the axis of symmetry will appear as a periodic oscillation "damped" by increasing uniformity of the spread of the tracer particles in the batch with superimposed random pulsations due to the flow of the fluid.

In the preceding communication it was shown that on the basis of the analysis of the random motion of a single particle one can describe, under certain assumptions, the behaviour of a set of such particles, *i.e.* also their concentration. The concentration changes of the tracer solute characterized above shall be therefore simulated by describing a suitably selected single tracer particle on the mentioned straight line. The straight line is taken to be the  $x$  axis directed toward the bottom of the vessel. The origin of the  $x$  axis is at the point of intersection with the horizontal plane of symmetry of the impeller (Fig. 1).

Following are the simplifying assumptions enabling quantitative description of this motion: *A1* The tracer particle moving within the liquid is subject to the action of these forces: *a)* force of friction, directly proportional to its velocity and opposite in direction; *b)* central force, induced by mutual action of the impeller and the reaction of the wall of the vessel, directly proportional to the position of the particle; *c)* random force, proportional to the Wiener's process<sup>2</sup>. The coefficients of proportionality for the above forces are constants for given conditions of mixing.

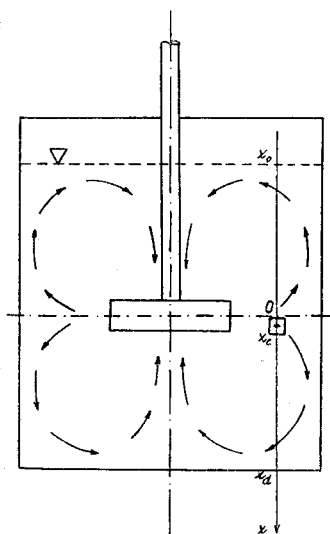


FIG. 1

Sketch of Motion of Tracer Particle in Mixed Batch

0 Origin of axis  $x$  (point of intersection with the horizontal plane of symmetry of the impeller),  $x_0$  injection point for tracer solute,  $x_c$  coordinate of position of the detector (center),  $x_d$  point of intersection of axis  $x$  and bottom.

*Note:* On the basis of the above description of the spread of the tracer solute in the batch and the previous communication<sup>1</sup> the force defined sub *b*) may be thought to bring about the circulatory flow of the fluid carrying the tracer solution. The force of friction, defined sub *a*) characterizes the existence of the velocity profile within this stream and hence the contribution of lateral mixing to the spread of the tracer solute while the random force sub *c*) represents a contribution of the turbulent transport. *A2* The motion of the particle with respect to liquid is negligible in comparison with that induced by the above defined random force. *Note:* As follows from the earlier considerations<sup>1</sup> the assumption expresses the fact that molecular diffusion is negligible with respect to the turbulent transport. The motion of the particle may then be identified with the motion of the fluid that surrounds it. *A3* The velocity of particle's motion is initially zero. *A4* The probability that the particle escapes in the course of the process from the system (*i.e.* appears outside the line segment given by  $x_0$  and  $x_a$ ) is taken to be negligibly small but non-zero with respect to the reverse process.

With the aid of the first two assumptions the stochastic differential equations describing the motion of the tracer particle under consideration may be written as<sup>1,3</sup>

$$\begin{aligned}dV(t) &= [-aV(t) - bX(t)] dt + cdW(t), \\dX(t) &= V(t) dt.\end{aligned}\quad (1)$$

Here  $V$  and  $X$  designate velocity and position of the particle taken generally to be random functions of time,  $t$ .  $W$  designates Wiener's process. The symbols  $a$ ,  $b$  and  $c$  are positive coefficients, constant under given conditions of mixing (*i.e.* the frequency of revolution of the impeller, geometrical arrangement *etc.*).

The random functions in Eqs (1) and (2) may be thought to be Markov's processes<sup>4</sup> and the appropriate transitive probability density may be written as

$$\begin{aligned}f'(x, v; t|x^0, v^0) &= \\&= \lim_{\substack{\Delta x \rightarrow 0 \\ \Delta v \rightarrow 0}} \frac{1}{\Delta x \Delta v} P\{x \leq X(t) < x + \Delta x, v \leq V(t) < v + \Delta v | X(0) = x^0, V(0) = v^0\}.\end{aligned}\quad (3)$$

For this function one can find the following Kolmogorov's diffusion equation<sup>5</sup>

$$\frac{\partial f'}{\partial t} + v \frac{\partial f'}{\partial x} - \frac{\partial}{\partial v} \{[(\alpha_1^2 + \alpha_2^2)x + 2\alpha_1 v] f'\} - 2\sigma^2 \alpha_1 (\alpha_1^2 + \alpha_2^2) \frac{\partial^2 f'}{\partial v^2} = 0 \quad (4)$$

the coefficients of which ( $\alpha_1$ ,  $\alpha_2$ ,  $\sigma$ ) are associated with the coefficients of the differential equation (1) and (2) by

$$a = 2\alpha_1, b = \alpha_1^2 + \alpha_2^2, c^2 = 4\sigma^2 \alpha_1 (\alpha_1^2 + \alpha_2^2). \quad (5)$$

With regard to the initial position (the point  $x_0$ ) and the third assumption the initial condition for solving Eq. (4) may be written as

$$f^0(x^0, v^0) = \delta(x^0 + x_0) \delta(v^0), \quad (6)$$

where the symbol  $\delta(\cdot)$  designates the Dirac impulse function. Using the fourth assumption the boundary conditions on the limits of the finite interval need not be considered. Accordingly, we shall assume the usual behaviour of the probability density for the argument growing above all limits. Namely, the function  $f'(\cdot)$  and its first derivative vanish.

It can be proven that solution of Eq. (4) under these conditions is the two-dimensional normal distribution:

$$\begin{aligned} f(x, v; t) &= \iint_{-\infty}^{+\infty} f'(x, v; t | x^0, v^0) \delta(x^0 + x_0) \delta(v^0) dx^0 dv^0 = \\ &= \frac{1}{2\pi(h_{xx}h_{vv} - h_{xv}^2)^{1/2}} \exp \left\{ -\frac{h_{vv}(x - \bar{x})^2 - 2h_{xv}(x - \bar{x})(v - \bar{v}) + h_{xx}(v - \bar{v})^2}{2(h_{xx}h_{vv} - h_{xv}^2)} \right\} \end{aligned} \quad (7)$$

the parameters of which are functions of time and the initial conditions

$$\left. \begin{aligned} \bar{x} &= -x_0 \exp(-\alpha_1 t) [\cos(\alpha_2 t) + (\alpha_1/\alpha_2) \sin(\alpha_2 t)] \\ \bar{v} &= x_0 [(\alpha_1^2 + \alpha_2^2)/\alpha_2] \exp(-\alpha_1 t) \sin(\alpha_2 t) \end{aligned} \right\} \quad (8)$$

$$\left. \begin{aligned} h_{xx} &= \sigma^2 \left\{ 1 - [\exp(-2\alpha_1 t)/\alpha_2^2] \cdot \right. \\ &\quad \left. \cdot [\alpha_1^2 + \alpha_2^2 - \alpha_1^2 \cos(2\alpha_2 t) + \alpha_1 \alpha_2 \sin(2\alpha_2 t)] \right\} \\ h_{xv} &= \sigma^2 [\alpha_1(\alpha_1^2 + \alpha_2^2)/\alpha_2^2] \exp(-2\alpha_1 t) [1 - \cos(2\alpha_2 t)] \\ h_{vv} &= \sigma^2 (\alpha_1^2 + \alpha_2^2) \left\{ 1 - [\exp(-2\alpha_1 t)/\alpha_1^2] \cdot \right. \\ &\quad \left. \cdot [\alpha_1^2 + \alpha_2^2 - \alpha_1^2 \cos(2\alpha_2 t) - \alpha_1 \alpha_2 \sin(2\alpha_2 t)] \right\} \end{aligned} \right\} \quad (9)$$

The motion of the tracer particle along the considered straight line is thus fully described.

In the previous communication<sup>1</sup> it was shown that the found probability density,  $f(\cdot)$ , is directly proportional to the scalar quantity  $q(x, v, t)$  which shall be now regarded to be concentration:

$$q(x, v, t) f_v(v; t) = k f(x, v; t) \quad (10)$$

$f_v(\cdot)$  is the marginal probability density of the function  $V(t)$  and  $k$  is the proportionality constant. It was further shown that as long as  $V(t)$  is a random function of time the concentration  $q(x, V(t), t) = Q(x, t)$  is also a random function of time and space.

The expected value of this function can be found easily:

$$E\{Q(x, t)\} = \int_{-\infty}^{+\infty} q(x, v, t) f_v(v; t) dv = k \int_{-\infty}^{+\infty} f(x, v; t) dv.$$

Substituting into this expression for  $f(\cdot)$  from Eq. (7) we obtain after integration

$$E\{Q(x, t)\} = \frac{k}{(2\pi h_{xx})^{1/2}} \exp\left[-\frac{(x - \bar{x})^2}{2h_{xx}}\right], \quad (11)$$

where the quantities  $\bar{x}$  and  $h_{xx}$  are given by the first equations of the sets (8) and (9).

In order that we may confront this result suitably with the experimental data we shall introduce a dimensionless concentration  $Z(x_c, t)$  at the point  $x_c$ , *i.e.* location of the detector (Fig. 1):

$$Z(x_c, t) \equiv \frac{Q(x_c, \infty) - Q(x_c, t)}{Q(x_c, \infty) - Q(x_c, 0)} \quad (12)$$

and express this quantity explicitly as a function of time.

If we exclude from our consideration direct injection of the tracer solute at the beginning of the process into the detector the value of  $Q(x_c, 0)$  will always equal zero. The function  $Q(x_c, \infty)$  is independent of velocity, as may be apparent from the second expression (9), and therefore not a random function. Instead, as follows from Eq. (11), it equals

$$Q(x_c, \infty) = \lim_{t \rightarrow \infty} E\{Q(x, t)\} = \frac{k}{(2\pi\sigma)^{1/2}} \exp\left(-\frac{x_c^2}{2\sigma^2}\right). \quad (13)$$

For the expected value of the dimensionless concentration we finally obtain by substituting from Eqs (11) and (13) into (12) the relation

$$E\{Z(x_c, t)\} = 1 - E\{Q(x_c, t)/Q(x_c, \infty)\} = 1 - \frac{1}{\eta} \exp\left[-\frac{(\alpha_4 + \alpha_3\xi)^2}{2\eta^2} + \alpha_4^2\right], \quad (14)$$

where the parameters  $\alpha_3$  and  $\alpha_4$  are defined by

$$\alpha_3 \equiv x_0/(2\sigma)^{1/2}, \quad \alpha_4 \equiv x_c/(2\sigma)^{1/2}. \quad (15)$$

The expressions

$$\xi \equiv -\bar{x}/x_0, \quad \eta^2 \equiv h_{xx}/\sigma^2 \quad (16)$$

are, as follows from Eqs (8) and (9), dimensionless functions of time and the parameters  $\alpha_1$  and  $\alpha_2$ .

Eq. (14) thus describes under the above simplifying assumptions, the dependence of the expected value of the dimensionless concentration on time. It contains four parameters  $\alpha_k$  ( $k = 1, \dots, 4$ ) the values of which must be determined empirically.

## EXPERIMENTAL

*Experimental set-up.* The validity of Eq. (14) was tested experimentally in a perspex glass cylindrical vessel 0.29 m in diameter with four symmetrically located radial baffles 0.03 m wide. The clear liquid height was equal to the diameter of the vessel.

Two turbine impellers of the diameter ratio  $d/D$  equal  $1/3$  and  $1/4$  were used. The frequency of revolution of the impellers ranged between  $1.67$  and  $8.33 \text{ s}^{-1}$  and was held constant to  $\pm 2\%$ . The batch was distilled water with a small amount of sodium chloride. The temperature of the batch was held constant in the range  $20.0 \pm 0.1^\circ\text{C}$ . A glass cooling coil was placed in the vessel symmetrically around the axis of symmetry of the vessel in one of the experimental runs.

*Experimental method.* The observed quantity — concentration of sodium chloride in water — was detected by measuring electric conductivity of the solution by the compensation method worked out by Landau and Procházka<sup>6</sup>. The samples of the concentrated solution were added by a syringe onto the liquid level. The time of injection did not exceed 3 s. Also the time of observation of the recorded quantity and preliminary processing were the same as in the already cited paper<sup>6</sup> with the only difference that Eq. (12) was used for calculating the dimensionless concentration and the recorded quantity was sampled in equidistant time intervals.

The division of the time axis in one experimental run was always such that the number of these intervals,  $p$ , be always greater than 15. For  $Q(x_c, \alpha)$  in Eq. (12) we substituted the concentration at the time  $t_p$ , i.e. its final value which practically did not change with time.

*Data processing.* Each experimental run at given conditions was usually repeated 20 times, this means generally  $m$  realizations of the random function of time,  $Z(x_c, t)$ , in equidistant time intervals. The  $i$ -th realization ( $i = 1, \dots, m$ ) at a time  $t_j$  is designated as  $z_{ij}$ . The experimental estimate of the expected value  $E\{Z(x_c, t_j)\}$  is the mean of  $m$  realizations:

$$\bar{z}_j = \frac{1}{m} \sum_{i=1}^m z_{ij} \quad (17)$$

and the estimate of the variance,  $\text{Var}\{Z(x_c, t_j)\}$ , the quantity

$$s_j^2 = \frac{1}{m-1} \sum_{i=1}^m (z_{ij} - \bar{z}_j)^2. \quad (18)$$

To estimate the parameters  $\alpha_k$  in Eq. (14) we used nonlinear regression for the sequence  $\bar{z}_j$  weighted by appropriate estimates of the variance  $s_j^2$  (ref.<sup>7</sup>). The Gauss-Seidell<sup>8</sup> iteration method was used for the calculation. The initial estimates of the parameters  $\alpha_k$  were determined by qua-

litative comparison of the graphical records of the experimental courses of the sequence  $\bar{z}_j$  with that defined by Eq. (14) for *a priori* selected values of the parameters  $\alpha_k$ . This approach facilitated rapid convergence of the iteration.

Substitution of the obtained values of  $\alpha_k$  into Eq. (14) yielded the expected values of the function  $E\{Z(x_c, t)\}$  designated as  $S(t)$ .

*A criterion of the fit of experimental and model data.* The commonly used tests such as *e.g.* the *F*-test could not be used for comparison of the experimental estimates of the mean dimensionless concentration  $\bar{z}_j$  with the corresponding estimates of the expected concentrations  $S(t_j)$  for two reasons. First, the function,  $S(t_j)$  is not linear (even approximately not) with respect to the parameters  $\alpha_k$ , and secondly, the function  $Z(x_c, t)$  cannot be regarded as normal (not even approximately). As follows from Eq. (12) the latter function is not even symmetric as the concentration  $Q(x_c, t)$  takes only positive values.

Accordingly the approach was following: The function  $S(t)$  was assigned the confidence limits using the Tchebyshev<sup>9</sup> nonequality in which the expected value and the variance of the function  $Z(x_c, t)$  were replaced by their experimental estimates (Eqs (17) and (18)). Namely:

$$P\{|S(t_j) - \bar{z}_j| \leq \beta s_j / \sqrt{m}\} \geq 1 - 1/\beta^2. \quad (19)$$

The value of  $\beta$  was set equal to two<sup>10</sup>. A typical course of the function  $S(t)$  with the appropriate confidence limits and the values of  $\bar{z}_j$  is shown in Fig. 2.

In accord with Eq. (19) it was assumed that the model concept agrees with sufficient accuracy with the experimental data unless the ratio of the values  $z_j$  at given experimental conditions satisfying the nonequality in the brackets on the left hand side of the last expression is smaller than  $1 - 1/\beta^2$  (*i.e.* for the chosen  $\beta$  smaller than 75%).

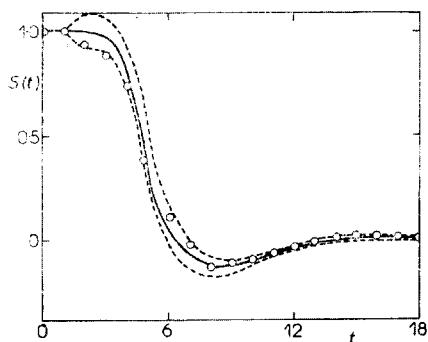


FIG. 2

Typical Course of Function  $S(t)$

— Function  $S(t)$ , ---- confidence limits, ○ experimentally determined means  $\bar{z}_j$  time  $t$  in s.

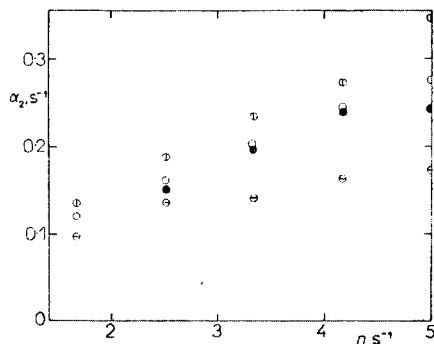


FIG. 3

Parameter  $\alpha_2$  as a Function of Frequency of Revolution of Impeller

○  $D/d = 3$ , cooling coil; ○  $D/d = 3$ , no coil; ⊙  $D/d = 4$ , no coil, ● values of similarly defined parameter<sup>11</sup> characterizing circulation of a tracer particle in the batch  $D/d = 3$ , no coil.

*Note:* Replacement of the probability characteristics in the nonequalities (19) by their estimates is clearly incorrect and impairs the reliability of the given method of comparison. This reliability apparently increases with the number of realizations,  $m$ .

## DISCUSSION

The model presented above, just like any other model, is capable of describing the investigated process only to some extent, or within a certain accuracy. The goodness of fit as a rule deteriorates with the simplification of the model. From this viewpoint it is possible to formulate a sequence of individual concepts simplifying the real situation:

1) The use of the continuous Markov's processes for description of the examined process leads to the partial differential equation of the parabolic type.

2) The considerations regarding the use of the unidimensional model (with respect to spatial coordinates) enables the number of the variables in the above equation to be reasonably decreased.

3) The assumption neglecting molecular diffusion (assumption A2) further simplifies the differential equation.

4) The assumptions regarding the acting forces (assumptions A1a, b, c) determine the form of the coefficients in this equation permitting thus an analytical solution to be obtained.

5) The assumptions regarding the initial and the boundary conditions (A3 and A4) confine on one hand the number of parameters of the solution and, on the other hand permit the fundamental solution to be obtained, *i.e.* relatively simple form of the resulting equation.

Such extensive set of simplifying assumptions can, of course, lead at best to a semi-empirical result which must be tested under various experimental conditions. Nevertheless, it will be shown that certain physical meaning following from the model remains preserved.

As has been mentioned, the motion of the tracer solute in the batch is simulated by unidimensional damped oscillation superimposed by random pulsations characterized by the last term on the right hand side of Eq. (1). With respect to the second of Eq. (5) the parameter  $\alpha_2$  is angular frequency of this oscillation as may be readily apparent from Eqs (1) and (2) if the last term is omitted. The parameter  $\alpha_2$  thus characterizes the circulation of the tracer solute together with the batch within the system. It may be therefore assumed that  $\alpha_2$  will depend on the conditions causing the circulation, *i.e.* in the first place the frequency of revolution of the impeller. As it further follows from Eqs (8) and (9) physical dimension of  $\alpha_2$  is time raised to minus first power. From comparison with the dimension of the frequency of revolution of the impeller it can be speculated that  $\alpha_2$  is proportional to  $n$ .



As may be seen from Fig. 3 the experimental results confirm this speculation and indicate effects of other factors too, which stimulate the circulation: Increasing size of the impeller and the presence of the cooling coil within the system which acts as a stream directing device.

From this standpoint appears also as remarkable the result of comparison with experimental measurement of the circulation of liquid in a similar apparatus by means of a tracer particle<sup>11</sup>. The parameter  $\omega$  in the cited paper has been introduced on the basis of a similar but simpler model concept as that in this work characterizing the circulation of the tracer particle and hence the liquid. Its values were plotted also in Fig. 3 as a function of the frequency of revolution of the impeller and well agree with the corresponding values of the parameter  $\alpha_2$ .

This fact, although so far verified in a rather narrow region, supports the consideration of possible description of the transfer of scalar quantities on the basis of independent experiments using tracer particles.

The agreement between the proposed function, Eq. (14), and the experimental data for 15 experimental conditions of this work is evidenced, provided that we accept the criterion proposed in the preceding paragraph, by the fact that 89% of the experimental data falls within the confidence limits calculated from Eq. (19). In none of the experimental conditions used did this fraction drop below the chosen value of 75%.

*Note:* The results for all experimental conditions were plotted by a computer and these plots qualitatively fully confirm the above facts. Typical such plot is shown in Fig. 2.

It can be thus concluded that although the experiments represent only a first stage of testing, the proposed general approach<sup>1</sup> seems prospective for description of the transfer of a scalar quantity in a nonideal mixer under a random character of the flow of the batch.

*The authors wish to thank Mrs L. Formanová for careful experimenting and evaluation of the data.*

#### LIST OF SYMBOLS

$a$	coefficient of friction force ( $s^{-1}$ )
$b$	coefficient of central force ( $s^{-1}$ )
$c$	coefficient of random force ( $m s^{-3/2}$ )
$D$	diameter of vessel (m)
$d$	diameter of impeller (m)
$f$	probability density
$h$	second central moment
$k$	proportionality constant in Eq. (10) ( $kg m^{-2}$ )
$m$	number of realization of random function
$n$	frequency of revolution of impeller ( $s^{-1}$ )

$p$	number of time intervals in a single experimental run
$Q$	volume concentration (random function) ( $\text{kg m}^{-3}$ )
$q$	volume concentration ( $\text{kg m}^{-3}$ )
$S$	estimate of expected value of dimensionless concentration
$s^2$	experimental estimate of variance
$t$	time (s)
$v$	velocity of tracer particle (random function) ( $\text{m s}^{-1}$ )
$v$	velocity ( $\text{m s}^{-1}$ )
$W$	Wiener's process (random function) ( $\text{s}^{1/2}$ )
$X$	position of tracer particle (random function) (m)
$x$	coordinate of position (m)
$Z$	dimensionless concentration (random function)
$z$	realization of dimensionless concentration
$\alpha$	model parameter
$\beta$	constant of significance level
$\delta$	Dirac impulse function
$\sigma^2$	stationary variance of position of tracer particle ( $\text{m}^2$ )

## Subscripts

$c$	detector
$d$	bottom of vessel
$i$	sequence index of realization of random function
$j$	element of sequence of time intervals
$k$	sequence index of parameter alpha
$o$	injection point
$p$	last element of sequence of time intervals
$x$	position of tracer particle
$v$	velocity of tracer particle

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Translated by V. Staněk.