CERTAIN PROBLEMS WITH THE APPLICATION OF STOCHASTIC DIFFUSION PROCESSES FOR THE DESCRIPTION OF CHEMICAL ENGINEERING PHENOMENA. RELATIONS BETWEEN DIFFERENT TYPES OF DIFFUSION EQUATIONS

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Received December 4, 1990
Accepted September 23, 1991

The dependence is discussed between the "classical" diffusion equation commonly used in chemical engineering and the stochastic differential equations which describe this diffusion from the point of view of micromotion of individual particles. The resulting equations can be useful above all for the modelling of more complex diffusion processes.

In preceding papers[1-3], some problems were pointed out arising on applying the mathematical theory of random processes[4-6] for the description of transport processes used in chemical engineering. The differences were shown in the record of the Kolgomorov and "classical" diffusion equation which existed in case that the diffusion coefficients in the equations are functions of spatial coordinates[1].

In addition the works[5-8] were cited referring to the relations between the diffusion equations and the stochastic differential equations and to the fact that different forms of the record of diffusion equations depend on the different definitions of stochastic integral. A new definition of the stochastic integral was proposed[2] which, in some cases, makes it possible to record the "classical" form of diffusion equation used in chemical engineering for the description of mass and heat transfer.

In the next paper[3], some additional problems were pointed out arising from the record of diffusion equations in curvilinear coordinates. Among others also the complication of conditions is concerned which make it possible to record in this case the "classical" diffusion equation on the basis of stochastic approach.

In the present contribution, the conditions mentioned are given in more detail; as the most general case, their record in orthogonal curvilinear coordinates is considered. The cases are presented in which we succeeded in finding the analytical solution. To be able to discuss the different forms of diffusion equations and relations between them we shall write down the definition of stochastic integral in a generalized form first and then the relations between the single forms of stochastic differential equations.

"Generalized" Record of Stochastic Differential Equation

In preceding paper[2], the "generalized" stochastic integral was defined – in somewhat different designation – by relation (*23.2*)* as

$$\int_{t_a}^{t_b} [\boldsymbol{G}(\boldsymbol{X}(t), t) \,.\, \mathrm{d}\boldsymbol{W}(t)]^{\alpha} =$$

$$= \lim_{\varrho \to 0} \sum_{k=0}^{n-1} \boldsymbol{G}(\boldsymbol{X}(t_k) + \alpha\,\Delta\boldsymbol{X}_k, t_k + \alpha\,\Delta t_k) \,.\, \Delta\boldsymbol{W}_k \quad [0 \leqq \alpha \leqq 1]\,, \tag{1}$$

where α is the constant which can acquire values in the given interval. $\boldsymbol{X}(t)$ denotes the random vector function of deterministic argument t whose physical meaning is time. $\boldsymbol{G}(\boldsymbol{x}, t)$ is the second-order tensor whose single components are in general deterministic functions of spatial coordinates designated here by the position vector $\boldsymbol{x}$ and explicitly also by time. Function $\boldsymbol{W}(t)$ is the multidimensional Wiener process – random function of time – whose probability density is determined by the relation (compare relation (*3.2*))

$$\frac{\partial^n}{\prod_{i=1}^{n} \partial w_i} P\{\bigcap_{i=1}^{n} (W_i(t) < w_i)\} = (2\pi t)^{-n/2} \exp\left(-\sum_{i=1}^{n} w_i^2/2t\right). \tag{2}$$

The increments of quantities in Eq. (*1*) are defined by the relations

$$\Delta\boldsymbol{X}_k = \boldsymbol{X}(t_{k+1}) - \boldsymbol{X}(t_k)\,; \quad \Delta\boldsymbol{W}_k = \boldsymbol{W}(t_{k+1}) - \boldsymbol{W}(t_k)\,; \quad \Delta t_k = t_{k+1} - t_k \tag{3}$$

and $\varrho = \max \Delta t_k$. The sequence of single values of arguments is given by the relations $t_a = t_0 < t_1 < \cdots < t_k < t_{k+1} < \cdots < t_n = t_b$. Full stop between symbols $\boldsymbol{G} \,.\, \boldsymbol{W}$ denotes the scalar (inner) product.

The fundamental – mathematically correct – definition of stochastic integral is the Ito definition (see, e.g., ref.[7]) expressed by Eq. (*1*) for $\alpha = 0$ for only in this case the factors $\boldsymbol{G} \,.\, \Delta\boldsymbol{W}_k$ of each term of the sum on the right-hand side of the equation can be stochastically independent. (In ref.[2], the quantities which are connected with this Ito definition are denoted by superscript I.)

In literature[5–7] is further given the definition of the Stratonovich integral (for the value of $\alpha = 1/2$ in Eq. (*1*)); the author[9] himself stems here from the Ito definition.

* References to the relations in foregoing papers[1–3] will be designated in the form (*K*.I) where *K* stands for the number of relation and I for the reference number in the present list of references.

(The corresponding quantities connected with the Stratonovich definition are designated by superscript S in ref.[2].) This procedure was generalized[2], and it is possible to show easily that the relation between the generalized definition of the stochastic integral and the Ito definition is given by the equation

$$\int_{t_a}^{t_b} [\mathbf{G}(\mathbf{X}(t), t) \, . \, \mathrm{d}\mathbf{W}(t)]^\alpha = \int_{t_a}^{t_b} [\mathbf{G}(\mathbf{X}(t), t) \, . \, \mathrm{d}\mathbf{W}(t)]^0 + \alpha \int_{t_a}^{t_b} \mathbf{j}(\mathbf{X}(t), t) \, \mathrm{d}t \,, \qquad (4)$$

where the vector of "semidiffusion" flux $\mathbf{j}$ is given by the relation (compare (*15.2*))

$$\mathbf{j}(\mathbf{X}(t), t) = [\mathbf{G}^+(\mathbf{X}(t), t) \, . \, \nabla] \, . \, \mathbf{G}^+(\mathbf{X}(t), t) \, . \qquad (5)$$

Symbol ∇ denotes the Hamilton differential operator and $\mathbf{G}^+$ tensor transposed with respect to tensor $\mathbf{G}$. Square brackets determine the order of operations. The different expressions for the stochastic integral are conditioned by the fact that the difference of the Wiener process, $\Delta \mathbf{W}_k$, converges to zero more slowly than the time interval Δt_k.

The proposed record of stochastic integral makes it possible to get a generalized record of stochastic differential equation which will be given here in the integrated form

$$\mathbf{X}(t) = \mathbf{y} + \int_\tau^t \mathbf{v}^\alpha(\mathbf{X}(s), s) \, \mathrm{d}s + \int_\tau^t [\mathbf{G}(\mathbf{X}(s), s) \, . \, \mathrm{d}\mathbf{W}(s)]^\alpha \, ; \qquad (6)$$

$\mathbf{y}$ denotes the initial condition of solution, i.e., the value of random function $\mathbf{X}$ at instant τ. Deterministic vector function $\mathbf{v}^\alpha$ is often called the drift velocity and the first integral on the right-hand side of the relation is a common integral in the Riemann sense. In order that the solutions $\mathbf{X}(t)$ for different definitions of the second integral may be identical (in the stochastic sense), the drift velocity must acquire different expressions. It follows from Eqs (*4*) and (*6*) that the relation

$$\mathbf{v}^\alpha(\mathbf{X}(t), t) = \mathbf{v}^\beta(\mathbf{X}(t), t) + (\beta - \alpha) \mathbf{j}(\mathbf{X}(t), t) \, , \quad [0 \leqq \alpha, \beta \leqq 1] \qquad (7)$$

holds between these expressions.

The given relations may be of importance for the stochastic modelling of diffusion processes in terms of computers; it is reported[10] that the Stratonovich form of stochastic integral is suitable for this purpose.

In diffusion processes, the random function $\mathbf{X}(t)$ determines the position of diffusing particle in the space. Its general probabilities characteristic is given by the transitive probability density

$$f = f(\mathbf{x}; t | \mathbf{y}; \tau) = \frac{\partial^n}{\prod_{i=1}^{n} \partial x_i} P\{ \bigcap_{i=1}^{n} (X_i(t) < x_i) | \mathbf{X}(\tau) = \mathbf{y} \} \, ; \quad [t > \tau] \, . \qquad (8)$$

In the braces the probability is written down expressing that the particle will occur at instant t in the region of space delimited by the inequalities on condition that at the initial instant τ it was localized at the point which is determined by position vector $\mathbf{y}$.

It is being proved in the literature[4-8] that in case of the Ito calculus, function f is the solution of the forward partial differential Kolgomorov equation (see relations (*24*.2) and (*25*.2)) where, for the drift velocity is inserted the more general expression from Eq. (*7*)

$$\partial f/\partial t + \nabla . (f\mathbf{v}^{\alpha}(\mathbf{x}, t) + \alpha f\mathbf{j}(\mathbf{x}, t)) - \tfrac{1}{2}\nabla . (\nabla . (\mathbf{B}(\mathbf{x}, t) f)) = 0 . \tag{9}$$

Diffusion tensor $\mathbf{B}$ is here given by the expression

$$\mathbf{B}(\mathbf{x}, t) = \mathbf{G}(\mathbf{x}, t) . \mathbf{G}^{+}(\mathbf{x}, t) ; \tag{10}$$

its matrix is therefore symmetrical and positive definite. Further we shall write down the divergence of this expression (see (*4*.3))

$$\nabla . \mathbf{B}(\mathbf{x}, t) = \mathbf{j}(\mathbf{x}, t) + \mathbf{k}(\mathbf{x}, t) , \tag{11}$$

where vector $\mathbf{j}$ is defined by Eq. (*5*) and vector $\mathbf{k}$ by the relation

$$\mathbf{k}(\mathbf{X}(t), t) = \mathbf{G}(\mathbf{X}(t), t) . [\nabla . \mathbf{G}(\mathbf{X}(t), t)] . \tag{12}$$

On inserting from Eq. (*11*) into Eq. (*9*), we obtain the "generalized" diffusion equation

$$\partial f/\partial t + \nabla . [f(\mathbf{v}^{\alpha}(\mathbf{x}, t) + (\alpha - 1/2)\mathbf{j}(\mathbf{x}, t) - 1/2\mathbf{k}(\mathbf{x}, t))] - $$
$$- 1/2\nabla . [\mathbf{B}(\mathbf{x}, t) . \nabla f] = 0 . \tag{13}$$

The solution of Eq. (*13*) is as well given by the unconditional probability density $p(\mathbf{x}, t)$ which is obtained from the initial distribution of random function $\mathbf{X}$ (see Eq. (*19*.1)):

$$p(\mathbf{x}; t) = \int f(\mathbf{x}; t|\mathbf{y}; \tau)\, p(\mathbf{y}; \tau)\, \mathrm{d}\mathbf{y} . \tag{14}$$

In case of the Stratonovich definition of stochastic integral (i.e., for $\alpha = 1/2$), the middle term of sum in the first brackets is vanishing and the last two terms can be added for

$$\nabla . [f\mathbf{k}(\mathbf{x}, t) + \mathbf{B}(\mathbf{x}, t) . \nabla f] = \nabla . [\mathbf{G}(\mathbf{x}, t) . (\nabla . \mathbf{G}(\mathbf{x}, t) f)] \tag{15}$$

holds; after inserting from this relation into Eq. (*13*), we obtain the usual expression for the Stratonovich form of diffusion equation[2,9].

In contribution[2], the "transport" diffusion equation was proposed for the case when $\alpha = 1$:

$$\partial f/\partial t + \nabla . [f\mathbf{v}^{1}(\mathbf{x}, t) + \tfrac{1}{2}f(\mathbf{j}(\mathbf{x}, t) - \mathbf{k}(\mathbf{x}, t))] - \tfrac{1}{2}\nabla . [\mathbf{B}(x, t) . \nabla f] = 0 . \tag{16}$$

(In the corresponding equations of the paper cited, the corresponding quantities were designated by superscript T.) The last term of this equation is, as to the order of differential operators, identical with the expressions used in differential equations for transport of heat and/or substance component. The solution of Eq. (*16*) therefore may be also the concentration of substance component for the transformation

$$c(\mathbf{x}, t) = kp(\mathbf{x}, t)/\sqrt{g(\mathbf{x})} \tag{17}$$

holds (see relation (*21*.3)).

Provided function c has the meaning of concentration, constant k is equal to the total amount of component, in case of temperature it is proportional to the enthalpy of fluid in the subspace considered. Symbol g denotes the determinant of metric tensor[11] (see *12*.3)) for the probability density – unlike temperature or concentration – is not transformed as an absolute scalar. In case of the Cartesian coordinates, the value of g is identically equal to unity. The components of tensor $\mathbf{B}$ in Eq. (*16*) can then be considered either as diffusion coefficients or thermal conductivity coefficients. This coefficient is often scalar, i.e., $\mathbf{B}(\mathbf{x}, t) = \mathbf{I}B(\mathbf{x}, t)$ where $\mathbf{I}$ is the identity tensor. In the simplest case B can be considered to be a scalar constant.

As it has been reported in foregoing papers[1-3], the fundamental problem of applying this mathematical theory in chemical engineering is the question which of the drift velocities is to be identified with the velocity of fluid in which the process takes place, which formally means to choose suitably parameter α in Eqs (*9*) or (*16*). At the same place, the view was expressed that this question cannot be apparently solved unambiguously, however, that in most chemical-engineering problems, Eq. (*16*) (with $\alpha = 1$) under the simultaneous validity of the condition (see Eq. (*8*.3))

$$\mathbf{j}(\mathbf{x}, t) = \mathbf{k}(\mathbf{x}, t) \tag{18}$$

is used.

In the following paragraph, the validity of this condition will be investigated in more detail.

Condition for the Record of "Classical" Diffusion Equation on the Basis of Notion of Stochastic Motion of Diffusing Particles

When recording stochastic equations (*6*) which describe the motion of diffusing particles, it is considered that the coefficients in these equations, i.e., functions $\mathbf{v}^{\alpha}(\mathbf{x}, t)$ and $\mathbf{G}(\mathbf{x}, t)$, are a priori known. Then it follows from condition (*18*) that not every function $\mathbf{G}(\mathbf{x}, t)$ makes it possible to write down the diffusion equation in the classical form.

When describing the transport processes, however, the coefficients of partial differential equations (*9*) or (*13*), $\mathbf{v}^{\alpha}(\mathbf{x}, t)$ and $\mathbf{B}(\mathbf{x}, t)$ are set (as found, e.g., by experiment), the symmetry of tensor $\mathbf{B}$ being usually considered. As it follows from Eq. (*10*), the last assumption is the necessary condition for the existence of a relation between the stochastic differential equations and the respective diffusion equations. The matrix of diffusion tensor must be further positive definite, which among others means that the values of main minors as well as the value of determinant of this matrix is in all cases positive[12].

For the record of corresponding stochastic (differential) equations is then, on the contrary, necessary to determine tensor **G**. It is to be emphasized that this problem is not usually unambiguous and that, therefore, more stochastic equations may correspond to one diffusion equation. It is then advantageous to choose from a series of possible stochastic equations such an equation in which the matrix of tensor **G** has as simple as possible form from the point of view of determining its elements.

Providing that the elements of matrix of tensor **B** are set, tensor **G** is not determined only by Eqs (*10*) unless this tensor is, e.g., symmetric as well. However, it is possible to make sure simply, e.g., by writing down condition (*18*) in Cartesian coordinates, that it is not fulfilled by the elements of matrix of symmetric tensor **G**. Therefore, $n(n+1)/2$ relations and further n equations follow generally from Eq. (*10*) and condition (*18*), respectively, for the determination of elements of the tensor **G** matrix for the set tensor **B**. To determine all the elements of the tensor **G**, the condition

$$n^2 = n(n+1)/2 + n \qquad (19)$$

must apparently hold, which is fulfilled for $n = 3$ only, therefore for three-dimensional problems. The one- or two-dimensional problems are overdetermined by the number of relations given by the last equation. However, we shall show below (see Appendix I) that in case of the scalar diffusion coefficient, $B(\mathbf{x}, t)$, (consequently even in case of one-dimensional problems), condition (*18*) is fulfilled automatically and so simply holds

$$G(\mathbf{x}, t) = \pm \sqrt{B(\mathbf{x}, t)}\,. \qquad (20)$$

For the two-dimensional problems, however, five equations are available for four elements of tensor **G** and therefore one constraint must hold between elements of matrix of tensor **B** which therefore cannot be set arbitrarily. Multidimensional problems (exceeding three-dimensional) would be underdetermined.

Thus, it is possible to draw the conclusion that in three-dimensional Euclidean space – on setting tensor **B** with symmetric and positive definite matrix – it is possible to determine the elements of matrix of tensor **G** for condition (*18*) to be fulfilled. From the concepts of stochastic motion of diffusing particles and application of the corresponding mathematical apparatus it is therefore possible, under the given conditions, always to derive the "classical" diffusion equation for the description of transport phenomena. The "transport" drift velocity (i.e., the case when parameter α equals unity) then can be identified with the velocity of fluid in which the mass or heat transfer takes place.

The finding of elements of matrix of tensor **G** is not, however, a simple problem. In preceding paper[3], condition *(18)* was written down in a sufficiently general form – i.e., in orthogonal curvilinear coordinates (Eq. *(28*.3)) which is given here in somewhat altered form

$$\sum_{\substack{i=1\\i\neq k}}^{n}\sum_{j=1}^{n} G_{ij}^{2}\frac{\partial}{e_i\,\partial z_i}\left(\frac{G_{kj}}{G_{ij}}\right) = 2\sum_{j=1}^{n}\sum_{\substack{i=1\\i\neq j}}^{n}\left[G_{kj}\left(G_{ii}\frac{\partial\ln e_i}{e_j\,\partial z_j} - G_{ji}\frac{\partial\ln e_j}{e_i\,\partial z_i}\right)\right] +$$

$$+\sum_{i=1}^{n}\left[B_{ii}\frac{\partial\ln e_i}{e_k\,\partial z_k} + B_{ik}\frac{\partial}{e_i\,\partial z_i}\ln\left(\frac{e}{e_i e_k}\right)\right],\quad [k = 1,\ldots n] \tag{21}$$

where, moreover,

$$B_{ij} = \sum_{k=1}^{n} G_{ik}G_{jk}\,,\quad [i = 1,\ldots,n;\, j = 1,\ldots,n] \tag{22}$$

follows from Eq. *(10)*.

The orthogonal curvilinear coordinates are designated by symbols z_i, symbols B_{ij} and G_{ij} are so-called natural coordinates of tensors[11], symbols e_i are roots of diagonal elements of matrix of fundamental tensor and are determined by the equations

$$e_i = \left[\sum_{k=1}^{n}\left(\frac{\partial x_k}{\partial z_i}\right)^2\right]^{1/2};\quad e = \prod_{i=1}^{n} e_i\,, \tag{23}$$

and x_k are Cartesian coordinates. In case of orthogonal coordinates, the relation $e = \sqrt{g}$ holds from which it would be possible to substitute into Eq. *(17)*.

The written equations make it possible to look for the solution for single types of diffusion processes (see also ref.[1]):

a) homogeneous and isotropic diffusion when the diffusion coefficient is a scalar constant: $\mathbf{B}(\mathbf{x}, t) = IB$; $B =$ const. The value G is in this case equal to square root of constant B. (From the point of view of modelling the stochastic processes with respect to the symmetry of the Wiener process in Eq. *(6)*, it is not decisive whether positive or negative value is chosen),

b) non-homogenous and isotropic diffusion – diffusion coefficient is a scalar function of spatial coordinates. It follows from Appendix I that even in this case, condition *(18)* is always fulfilled and function $G(\mathbf{x}, t)$ can be calculated from Eq. *(20)*,

c) homogeneous and anisotropic diffusion – this type of processes is characterized by diffusion tensor **B** whose all elements written down in the Cartesian coordinates are constants. In this case, condition *(18)* is fulfilled automatically and $n(n-1)/2$ elements of matrix of tensor **G** may be chosen arbitrarily. Then it is advantageous to arrange this matrix as triangular one with zero elements above the diagonal. It holds here above all the relation between elements of matrices of tensors **B** and **G**:

$$B_{ij} = \sum_{k=1}^{i} G_{ik} G_{jk}\,, \quad [i = 1, \ldots, n; j = 1, \ldots, n]\,. \tag{24}$$

Diagonal elements of matrix of tensor **G** can be determined in terms of simple expressions

$$G_{ii} = (D_i/D_{i-1})^{1/2}\,, \quad [i = 1, \ldots, n]\,, \tag{25}$$

where D_i are main minors of matrix of tensor **B** and $D_0 = 1$. In case of a positive definite matrix, they have always positive value[12]. The non-diagonal elements can be found from the recurrence relations

$$G_{ij} = (B_{ji} - \sum_{k=1}^{j-1} G_{jk} G_{ik})/G_{jj}\,, \quad [i = 2, \ldots, n; j < i]\,. \tag{26}$$

The first three main minors of matrix of tensor **B** have the form

$$D_1 = B_{11}\,; \quad D_2 = B_{11}B_{22} - B_{12}^2\,;$$

$$D_3 = B_{11}B_{22}B_{33} + 2B_{12}B_{13}B_{23} - (B_{11}B_{23}^2 + B_{22}B_{13}^2 + B_{33}B_{12}^2)\,. \tag{27}$$

In curvilinear coordinates, some components of tensors are a function of coordinates even in anisotropic homogeneous diffusion as it follows from the transformation relations

$$B'_{ij} = \sum_{k=1}^{n} \sum_{m=1}^{n} B_{km} \frac{\partial z_i}{\partial x_k} \frac{\partial z_j}{\partial x_m}\,; \tag{28}$$

components in curvilinear coordinates are designated by apostrophe.

d) non-homogeneous and anisotropic diffusion is the case when the components of tensor **B** are functions of spatial coordinates. In general, Eqs (*21*) and (*22*) hold here which are rather complicated. We succeeded in finding their analytical solution only for the two-dimensional case.

CONCLUSION

This contribution completes the series of preceding papers[1-3] so that it generalizes, complements and/or corrects the results included in them. It is proved in it above all that for every "classical" diffusion equation with the set factors **v** and **B**, i.e., the fluid velocity and diffusion tensor, there exists the corresponding stochastic (differential) equation stemming from the formerly[2] defined "transport" stochastic integral (i.e., for $\alpha = 1$). Two-dimensional problems are an exception which require a constraint between the set components of matrix of tensor **B**. We succeeded in explicit finding the general form of this condition (relation (*A.16*) in Appendix II).

As to a general solution for three-dimensional problems – even if it was shown that it exists and does not require a constraint among the elements of matrix of tensor $\mathbf{B}$ – we failed to find it even in the simplest cases of Cartesian or cylindrical coordinates. In some special cases it is possible to determine the elements of matrix of tensor $\mathbf{G}$, if the diffusion coefficient is scalar or when the elements of matrix of tensor $\mathbf{B}$ are not functions of spatial coordinates. In this last case it is suitable to choose the matrix of tensor $\mathbf{G}$ as triangular one.

In this connection it is necessary to give more precision and to correct some conclusions drawn in preceding paper. From reference[2], which unlike this work stems from the set factors $\mathbf{v}$ and $\mathbf{G}$, it is possible to draw conclusion that the considered problem has a solution in the case when the components of tensor $\mathbf{B}$ are a linear combination of three scalar functions of spatial coordinates (see relation (*34*.2)). In this case, the components of tensor $\mathbf{G}$ have the form $G_{ij} = c_{ij}h_j$, where h_j are the said scalar functions of spatial coordinates and c_{ij} are constants. However, it is necessary to define this conclusion with more precision so that it holds only for Cartesian coordinates. Likewise it is necessary to give precision to the statement that condition (*18*) is fulfilled for every diagonal matrix. This statement holds only in Cartesian coordinates; in general case, all diagonal elements must equal.

For the stochastic modelling of diffusion processes, however, it is not necessary, even in this complicated case, to determine the elements of matrix of tensor $\mathbf{G}$ in terms of condition (*18*). We can exploit the "generalized" diffusion equation (*13*) introduced in the first part of this work which is able to describe the "classical" diffusion[1] regardless of the fact how the corresponding stochastic integral (relation (*4*)) is defined. The sum in parentheses of the second term of Eq. (*13*) can be considered to be the fluid velocity and moreover, with respect to Eq. (*11*), to write

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{v}^{\alpha}(\mathbf{x}, t) + \alpha\mathbf{j}(\mathbf{x}, t) - \tfrac{1}{2}\nabla \cdot \mathbf{B}(\mathbf{x}, t) . \tag{29}$$

The corresponding stochastic equation (*6*) then takes the form

$$\mathbf{X}(t) = \mathbf{y} + \int_{\tau}^{t} [\mathbf{v}(\mathbf{X}(s), s) - \alpha\mathbf{j}(\mathbf{X}(s), s) + \tfrac{1}{2}\nabla \cdot \mathbf{B}(\mathbf{X}(s), s)]\, \mathrm{d}s + \int_{\tau}^{t} [\mathbf{G}(\mathbf{X}(s), s) \cdot \mathrm{d}\mathbf{W}(s)]^{\alpha} , \tag{30}$$

in which $\mathbf{v}$ and $\mathbf{B}$ are the set coefficients. Then it is not necessary to take account of condition (*18*), and the elements of matrix of tensor $\mathbf{G}$ can be easily found, e.g. on the assumption that this matrix is triangular, i.e., from Eqs (*24*) and (*27*). In this way it is therefore possible to model every "classical" diffusion equation regardless of the fact how the stochastic integral in the last term of Eq. (*30*) is defined. However, velocity $\mathbf{v}$ then need not generally be identical with drift velocity $\mathbf{v}^{\alpha}$ even if the stochastic integral in Eq. (*1*) is defined for any α from the given interval.

APPENDIX I

The record of condition (18) *for diagonal matrix of tensor* **B**. In the given case, the diagonal matrix is the simplest matrix of tensor **G**, and Eq. (*22*) reduces to the form

$$B_{ii} = G_{ii}^2 , \quad [i = 1, \ldots, n] . \tag{A.1}$$

Further, the numerator must be equal to denominator in each term of summation on the left-hand side of Eq. (*21*) and on differentiating, all the sum is equal to zero. Further, we introduce the designation

$$\frac{\partial \ln e_i}{e_k \, \partial z_k} = \psi_{ik} \tag{A.2}$$

on the right-hand side of Eq. (*21*) and on taking account of the second of Eqs (*23*) we can write down

$$2 \sum_{\substack{i=1 \\ i \neq j}}^{n} \sum_{j=1}^{n} (G_{ii}\psi_{ij} - G_{ji}\psi_{ji}) \, G_{kj} = \sum_{i=1}^{n} (B_{ii}\psi_{ik} - B_{ik}\psi_{ii} - B_{ik}\psi_{ik} + $$

$$+ \sum_{j=1}^{n} B_{ik}\psi_{ji}) \quad [k = 1, \ldots n] \tag{A.3}$$

In a diagonal matrix, the elements with unequal subscripts are zero, and therefore

$$2 \sum_{\substack{i=1 \\ i \neq k}}^{n} G_{ii} G_{kk} \psi_{ik} = \sum_{\substack{i=1 \\ i \neq k}}^{n} (B_{ii} + B_{kk}) \, \psi_{ik} , \tag{A.4}$$

and according to Eq. (*A.1*)

$$\sum_{\substack{i=1 \\ i \neq k}}^{n} (G_{ii} - G_{kk})^2 \, \psi_{ik} = 0 . \tag{A.5}$$

In case of orthogonal curvilinear coordinates, consequently, all the elements of diagonal matrix must be mutually equal.

APPENDIX II

Relation between components of diffusion tensor and calculation of components of stochastic tensor in two-dimensional problems. Let us assume that all three elements of matrix of diffusion tensor **B** of dimension 2 × 2 are given as functions of both the spatial coordinates and that they are such that this matrix is symmetric and positive definite. It is necessary to find four elements of stochastic tensor **G**.

Relations (*22*) will be only three in this case:

$$G_{11}^2 + G_{12}^2 = B_{11}\,; \quad G_{21}^2 + G_{22}^2 = B_{22}\,; \quad G_{11}G_{21} + G_{12}G_{22} = B_{12} = B_{21}\,. \tag{A.6}$$

Further, we shall apply Eqs (*21*) only to two coordinates; after rearranging we shall obtain, still on taking account of Eq. (*A.2*):

$$G_{21}^2 \frac{\partial}{e_i\,\partial z_i}\left(\frac{G_{11}}{G_{21}}\right) + G_{22}^2 \frac{\partial}{e_i\,\partial z_i}\left(\frac{G_{12}}{G_{22}}\right) =$$
$$= (-1)^i\,\psi_{ij}[2(G_{11}G_{22} - G_{12}G_{21}) + (B_{11} + B_{22})]\,; \quad [i, j = 1, 2;\, i \neq j]\,. \tag{A.7}$$

So we have five independent equations for four unknown functions; as it has been mentioned, a dependence must exist in this case between components of tensor **B**.

First we introduce new dimensionless functions by the equations

$$H_{ij} = G_{ij}/\sqrt{B_{ii}}\,; \quad \gamma = B_{12}/(B_{11}B_{22})^{1/2}\,, \quad [i, j = 1, 2]\,. \tag{A.8}$$

Relations (*A.6*) are simplified in this way to

$$H_{11}^2 + H_{12}^2 = 1\,; \quad H_{21}^2 + H_{22}^2 = 1\,; \quad H_{11}H_{21} + H_{12}H_{22} = \gamma\,. \tag{A.9}$$

Further, we substitute these dimensionless functions for the elements of matrix of tensor **G** in Eqs (*A.7*), differentiate and after algebraic rearrangements and on taking account of the last of Eqs (*A.9*) we get

$$H_{21}\frac{\partial H_{11}}{\partial z_i} - H_{11}\frac{\partial H_{21}}{\partial z_i} + H_{22}\frac{\partial H_{12}}{\partial z_i} - H_{12}\frac{\partial H_{22}}{\partial z_i} =$$
$$= \gamma\frac{\partial \varepsilon}{\partial z_i} + (-1)^i\,e_i\psi_{ij}[2(H_{11}H_{22} - H_{12}H_{21}) + (B_{11} + B_{22})/(B_{11}B_{22})^{1/2}]\,;$$
$$[i, j = 1, 2;\, i \neq j]\,. \tag{A.10}$$

We have introduced the designation

$$\varepsilon = \tfrac{1}{2}\ln(B_{22}/B_{11})\,. \tag{A.11}$$

Further we shall differentiate the first two equations (*A.9*), and gradually from these expressions, we shall substitute in each term on the left-hand side of Eq. (*A.10*). For instance, for the first term we have

$$H_{21}\frac{\partial H_{11}}{\partial z_i} = -H_{21}H_{12}\frac{\partial H_{12}}{\partial z_i}\Big/H_{11} = -H_{12}H_{21}\frac{\partial H_{12}}{\partial z_i}\Big/(1 - H_{12}^2)^{1/2} =$$

$$= -H_{12}H_{21}\frac{\partial}{\partial z_i}(\arcsin H_{12}) .$$

After analogous operations with all the terms on the left-hand side of Eqs ($A.10$) and on using the rules of subtraction of inverse goniometric functions, we obtain the relation

$$(H_{11}H_{22} - H_{12}H_{21})\frac{\partial}{\partial z_i}\arcsin(H_{22}H_{12} - H_{21}H_{11}) , \quad [i = 1, 2] .$$

Moreover, it follows from Eqs ($A.9$) that the first factor on the left-hand side of the last equation can be expressed as a function of γ:

$$H_{11}H_{22} - H_{12}H_{21} = (1 - \gamma^2)^{1/2} . \tag{A.12}$$

Equation ($A.10$) are divided by this factor and for the sake of brevity we introduce the designation

$$\lambda = \arcsin(H_{22}H_{12} - H_{21}H_{11}) ; \quad \varphi = \gamma/(1 - \gamma^2)^{1/2} ; \tag{A.13}$$
$$\varrho = 2 + (B_{11} + B_{22})/(B_{11}B_{22} - B_{12}^2) .$$

In the end we get two equations

$$\frac{\partial\lambda}{\partial z_i} = \varphi\frac{\partial\varepsilon}{\partial z_i} + (-1)^i e_i\psi_{ij}\varrho , \quad [i, j = 1, 2; i \neq j] \tag{A.14}$$

whose right-hand sides depend only on the set functions B_{ij}. To obtain an unambiguous solution, we differentiate each of them with respect to the second variable; we get

$$\frac{\partial^2\lambda}{\partial z_1\,\partial z_2} = \varphi\frac{\partial^2\varepsilon}{\partial z_1\,\partial z_2} + \frac{\partial\varphi}{\partial z_1}\frac{\partial\varepsilon}{\partial z_2} + \frac{\partial}{\partial z_1}(\psi_{21}e_2\varrho) ,$$
$$\frac{\partial^2\lambda}{\partial z_2\,\partial z_1} = \varphi\frac{\partial^2\varepsilon}{\partial z_2\,\partial z_1} + \frac{\partial\varphi}{\partial z_2}\frac{\partial\varepsilon}{\partial z_1} - \frac{\partial}{\partial z_2}(\psi_{12}e_1\varrho) . \tag{A.15}$$

The left-hand sides of both equations are equl each other; the first terms of right--hand sides as well; in order that also the second terms on the right-hand side may equal each other, the condition

$$\frac{\partial\varphi}{\partial z_1}\frac{\partial\varepsilon}{\partial z_2} + \frac{\partial}{\partial z_1}(\psi_{21}e_2\varrho) = \frac{\partial\varphi}{\partial z_2}\frac{\partial\varepsilon}{\partial z_1} - \frac{\partial}{\partial z_2}(\psi_{12}e_1\varrho) \tag{A.16}$$

must hold, which is the discussed dependence between the elements of matrix of tensor **B** in two-dimensional problems. Both equations ($A.15$) are then identical and their solution is

$$\lambda = \iint \left[\varphi \frac{\partial^2 \varepsilon}{\partial z_1 \, \partial z_2} + \frac{\partial \varphi}{\partial z_1} \frac{\partial \varepsilon}{\partial z_2} + \frac{\partial}{\partial z_1} (\psi_{21} e_2 \varrho) \right] \mathrm{d}z_1 \, \mathrm{d}z_2 \, . \qquad (A.17)$$

Furthermore we lay

$$\varkappa = \arcsin \gamma \, . \qquad (A.18)$$

Then it is possible to make sure easily that single functions H_{ij} are determined by the relations

$$H_{11} = \cos \alpha \, ; \quad \mathrm{H}_{12} = \sin \alpha \, ; \quad H_{21} = \sin \beta \, ; \quad H_{22} = \cos \beta \, , \qquad (A.19)$$

where

$$\alpha = (\varkappa + \lambda)/2 \, ; \quad \beta = (\varkappa - \lambda)/2 \, . \qquad (A.20)$$

Single elements of matrix of tensor **G** are established from the first equations (*A.8*).

Note: In case of the Cartesian coordinates, factors ψ_{ij} are identically equal to zero and condition (*A.16*) is then fulfilled if

$$\varphi = F(\varepsilon) \, , \qquad (A.21)$$

where F is an arbitrary function. The solution of Eq. (*A.17*) is then given by the relation

$$\lambda = \int F(\varepsilon) \, \mathrm{d}\varepsilon \, . \qquad (A.22)$$

Condition (*A.21*) can be written down as an explicit expression of dependence of non-diagonal element of matrix of tensor **B** on both the others

$$B_{12} = (B_{11} B_{22})^{1/2} \, \Phi(B_{22}/B_{11}) \, , \qquad (A.23)$$

where Φ is another arbitrary function; between functions F and Φ, naturally, there exists an unambiguous relation.

LIST OF SYMBOLS

B	diffusion tensor, $m^2 \, s^{-1}$
B	diffusivity, $m^2 \, s^{-1}$
B_{ij}	natural coordinate of diffusion tensor, $m^2 \, s^{-1}$
c	concentration of substance component, $kg \, m^{-3}$
D_i	main minor of matrix of tensor **B**
e	product of transformation coefficients ($e = \sqrt{g}$)
e_i	transformation coefficient
f	transitive probability density, m^{-n}
G	stochastic tensor, $m \, s^{-1/2}$

$\mathbf{G}^+$ tensor transposed to tensor $\mathbf{G}$, m $s^{-1/2}$
g determinant of metric tensor
$\mathbf{I}$ identity tensor
$\mathbf{j}$ vector defined by Eq. (*5*), m s^{-1}
$\mathbf{k}$ vector defined by Eq. (*12*), m s^{-1}
k proportionality constant in Eq. (*17*), kg
n rank of tensor matrix
p unconditional probability density, m^{-n}
t time, s
$\mathbf{v}$ fluid velocity, m s^{-1}
$\mathbf{v}^\alpha$ drift velocity, m s^{-1}
$\mathbf{W}$ (multidimensional) Wiener process, $s^{1/2}$
$\mathbf{X}$ position vector of diffusing particle — random function of time, m
$\mathbf{x}$ position vector of particle — variable of distribution function, m
$\mathbf{y}$ initial position of particle, m
z_i curvilinear orthogonal coordinate
α constant characterizing type of stochastic integral
τ initial time instant, s

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Translated by J. Linek.