Modeling of diffusion processes on physical and structural levels of materials

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Abstract
A possibility to use an integral operator for establishing the link between physical and structural levels of materials in modeling diffusion processes is considered. We show how to perform the transition from the stochastic description of motion of a system of points to the continuum description of diffusive profiles.

1 Introduction
Materials used industrially are complex multilevel systems. Analysis of these systems generally involves the consideration of their physical, structural and macroscopic levels (micro-, meso- and macrolevels). As a rule, for each level we can formulate a special equation that allows modeling the processes taking place in the material: molecular motions and interactions on the physical level, supermolecular formations and processes in the vicinity of inclusions in composites on the structural level, and the state of the body as a whole on the macroscopic level.

The considered processes can be studied separately on each level, which essentially simplifies their analysis. However, this possibility does not always exist. Such a modeling can be realized in the case when the points of higher level are the material regions that are representative (contain a great number of elements) and in homogeneous state. Under these conditions, the transition to state parameters of higher level can be performed by the averaging procedure. The studied volumes must be representative enough to exclude the fluctuation of parameters. The homogeneity of the state of these regions makes it possible to search the functional dependences on the higher level.

There is another way of establishing the link between processes on different levels. It suggests the construction of the mathematical operator for creation of process images on the higher level instead of the use of the hypothesis of

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representativeness and homogeneity of volumes. For composites, the transition from the structural level to the macroscopic one by the appropriate mathematical operator has been discussed in [1], [2]. This idea can also be used to realize the transition from the physical level to the structural one in modeling diffusion phenomena. In the present paper, we consider the simplest case that leads to the Fick law. The analysis of this case allows us to compare the results of numerical modeling of diffusion of a great number of particles with the process images on the level of continuous medium, to follow the disappearance of fluctuations and to find the most suitable form of the mathematical operator.

2 Modeling of diffusion of dissolved material constituents on physical level

We consider diffusion of \( n \) material points (particles). Their motion in the Euclidean space reproduces the diffusion of dissolved material constituents. It is assumed that the change in the position of the material point in space can be defined by Ito stochastic equations

\[
dx_n = v_n \, dt + b_n \, dz_n, \quad n = 1, \ldots, N, \tag{1}
\]

where \( x_n \) is the radius-vector of the \( n^{th} \) particle at time \( t \), \( v_n \) is the vector function, which defines the determinate component of particle motions in the Euclidean space, \( z_n \) are independent Wiener’s processes, and \( b_n > 0 \) is the scalar function characterizing the peculiarities of the chaotic motion of the \( n^{th} \) particle.

Let us clarify the obtained expressions. It is assumed, in the framework of this model, that particles move chaotically and, as a result, redistribute throughout the material, i.e., the mass transfer takes place. Constitutive equations are given as follows. The random motion can be represented as the most probable tendency (velocity \( v_n \)) and the chance deviations from it. The vector \( v_n \) is a mathematical expectation of the rate of change of the \( n^{th} \) particle space position. The deviations are described in the analysis of independent Wiener processes. The scatter value for random walks is given by the function \( b_n \). Our purpose in this work is to determine, in the framework of used mathematical models, conditions for the transition from the stochastic description of motion of points to the continuum description of mass transfer by the diffusion equation of a material constituent.

To derive the dependences we are interested in, the notion of a phase space \( \Gamma \) should be used, which is a set of possible values of the radius-vector components of particles. The phase space element \( d\Gamma \) is determined from

\[
d\Gamma = dx_1^1 \, dx_1^2 \, dx_1^3 \ldots dx_N^1 \, dx_N^2 \, dx_N^3 ,
\]

where \( x_i^j \) is the \( i^{th} \) coordinate of the radius-vector of \( n^{th} \) particle. To every system state there corresponds the phase space point \( \Gamma \). From here on the
symbol \( \psi \) will be used to denote the probability density of particles at time \( t \) in phase space \( \Gamma \) determined by the radius-vectors \( \mathbf{x}_1, ..., \mathbf{x}_N \)

\[
\psi = \psi(t, \mathbf{x}_1, ..., \mathbf{x}_N).
\]

The temporal variation of this density is defined by the Fokker — Planck equation [3], [4]

\[
\frac{\partial \psi}{\partial t} + \sum_{n=1}^{N} \nabla_{\mathbf{x}_n} \cdot \left( \psi \mathbf{v}_n \right) - \frac{1}{2} \sum_{n=1}^{N} \nabla_{\mathbf{x}_n}^2 : \left( b_n^2 \mathbf{I} \right) = 0,
\]

where

\[
\nabla_{\mathbf{x}_n} \ldots = \sum_{i=1}^{3} i_i \frac{\partial}{\partial x_n^i} \ldots, \quad \nabla_{\mathbf{x}_n}^2 \ldots = \nabla_{\mathbf{x}_n} \left( \nabla_{\mathbf{x}_n} \ldots \right),
\]

\( \mathbf{I} \) is a unit tensor, and \( \mathbf{i}_i \) are the basis vectors of a rectangular Cartesian coordinate system. It is clear that for phase space points at infinity the probability density \( \psi \) and its derivatives are equal to zero.

Numerical modeling of the motion of particles in space is limited to prescribing the random walks of particles \( \Delta \mathbf{x}_n \) within the time interval \( \Delta t \) according to the Gauss law \( \psi_n \) with the probability density \( \psi \) which has the form

\[
\psi_n = \prod_{i=1}^{3} \frac{1}{\sqrt{2\pi \Delta t b_n}} \exp \left( -\frac{(\Delta x_n^i - v_n^i \Delta t)^2}{2b_n^2 \Delta t} \right),
\]

where symbols \( v_n^i \) are the components of vectors \( \mathbf{v}_n \) in a rectangular Cartesian coordinate system.

### 3 Fluctuating and determinate mass densities of diffusing material constituent

In order to introduce continuum notions, we should perform the averaging procedure over the vicinity of the point in the Euclidean space. The simplest, yet not the best, way allowing the introduction of the mass density of a diffusing material constituent suggests the division of the number of particles in the vicinity of the studied point by the volume of this vicinity. This procedure gives the function dependent on the radius-vector of the Euclidean space, which pulsates as the radius-vector changes. The derivatives of this function with respect to coordinates can not be determined in this case. The region of averaging must be large enough to suppress these pulsations. The transition to the smoothed differential continuum notions only be possible following the corresponding hypothesis. In this section, we consider more formalized way of inserting the mass density of a diffusing constituent in our model.

Let us use the function \( \Pi \) to introduce the mesolevel notions. By this function one can evaluate the contribution of the \( n \)th material point having the radius-vector \( \mathbf{x}_n \) at time \( t \) to the state characteristics of the continuous medium.
at the point in the Euclidean space having the radius-vector \( \mathbf{x} \). We require that the function \( \Pi \) be continuous and have the continuous first derivative and the piece-wise continuous second derivative and become zero on moving apart from the point \( \mathbf{x} \) to the distance exceeding the value \( a_r \)

\[
\Pi(\mathbf{x} - \mathbf{x}_n) = 0 \quad \sqrt{(\mathbf{x} - \mathbf{x}_n) \cdot (\mathbf{x} - \mathbf{x}_n)} \geq a_r,
\]

satisfy the normalization condition

\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Pi(x^1_1 + x^2_2 + x^3_3) \, dx^1 \, dx^2 \, dx^3 = 1,
\]

and the requirement of independence of the space orientation of basis vectors

\[
\Pi(x^1_1 + x^2_2 + x^3_3) = \Pi \left( \mathbf{Q} \cdot (x^1_1 + x^2_2 + x^3_3) \right),
\]

where \( x^i \) are the coordinates of a rectangular Cartesian coordinate system, and \( \mathbf{Q} \) is the arbitrary rotation tensor. The function \( \Pi \) must be continuous and twice differentiated in order we can find the continuous twice differentiated parameters of the medium. The equations must satisfy the invariance requirement, i.e., they must be independent of the orientation of basis vectors. Hereafter, the function \( \Pi \) of the argument \( \mathbf{x} - \mathbf{x}_n \) will be denoted by the symbol \( \Pi_n \)

\[
\Pi_n = \Pi(\mathbf{x} - \mathbf{x}_n).
\]

Introduce the notion of the fluctuating density \( \tilde{\rho} \) for the diffusing material constituent by the following equality:

\[
\tilde{\rho}(t, \mathbf{x}) = m \sum_{n=1}^{N} \Pi_n,
\]

where \( m \) is the mass of one diffusing particle. Physically, the calculation of the density \( \tilde{\rho} \) involves averaging the particles over the volume of the material taking into account their distance from the considered point in the Euclidean space. The value \( \tilde{\rho} \) is the continuous and twice differentiated function, as the function \( \Pi \) is continuous and twice differentiated.

Introduce the notion of the density \( \rho \) of the diffusing constituent of the material by the expression

\[
\rho = m \int \sum_{n=1}^{N} \Pi_n \psi \, d\Gamma
\]

which is a mathematical expectation of the fluctuating density. Good agreement between \( \tilde{\rho} \) and \( \rho \) is only possible when the parameter \( a_r \) is sufficiently large and the distribution of particles in the spherical vicinity of the radius \( a_r \) of the considered point in the Euclidean space is almost uniform.
4 Derivation of the integral diffusion law from stochastic equations of particle motion

Consider the mathematical expression

\[ \int \left( \sum_{k=1}^{N} \Pi_k \right) \left[ \frac{\partial \psi}{\partial t} + \sum_{n=1}^{N} \nabla_{x_n} \cdot (\psi \mathbf{v}_n) - \frac{1}{2} \sum_{n=1}^{N} \nabla^2_{x_n} : \left( b_n^2 \psi \mathbf{I} \right) \right] d\Gamma = 0, \quad (5) \]

Its validity follows from (2), as the integrand function (in square brackets) is equal to zero. Let us rearrange equation (5) using three identities. The first can be derived based on the time independence of the function \( \Pi_k \)

\[ \int \left( \sum_{k=1}^{N} \Pi_k \right) \frac{\partial \psi}{\partial t} d\Gamma = \int \frac{\partial}{\partial t} \left( \sum_{k=1}^{N} \Pi_k \psi \right) d\Gamma. \]

The second is a consequence of vanishing of the probability density of state \( \psi \) at infinity of the phase space \( \Gamma \).

\[ \int \left( \sum_{k=1}^{N} \Pi_k \right) \nabla_{x_n} \cdot (\psi \mathbf{v}_n) d\Gamma = \]

\[ = \int \nabla_{x_n} \cdot \left[ \left( \sum_{k=1}^{N} \Pi_k \right) \left( \psi \mathbf{v}_n \right) \right] d\Gamma - \int \nabla_{x_n} \left( \sum_{k=1}^{N} \Pi_k \right) \cdot (\psi \mathbf{v}_n) d\Gamma = \]

\[ = - \int \nabla_{x_n} \left( \sum_{k=1}^{N} \Pi_k \right) \cdot (\psi \mathbf{v}_n) d\Gamma. \]

The last is derived from the expression

\[ \int \left( \sum_{k=1}^{N} \Pi_k \right) \nabla^2_{x_n} : \left( b_n^2 \psi \mathbf{I} \right) d\Gamma = \]

\[ = \int \nabla_{x_n} \cdot \left[ \left( \sum_{k=1}^{N} \Pi_k \right) \nabla_{x_n} \cdot \left( b_n^2 \psi \mathbf{I} \right) \right] d\Gamma - \]

\[ - \int \nabla_{x_n} \left( \sum_{k=1}^{N} \Pi_k \right) \cdot \nabla_{x_n} \cdot \left( b_n^2 \psi \mathbf{I} \right) d\Gamma = \]

\[ = - \int \nabla_{x_n} \left( \sum_{k=1}^{N} \Pi_k \right) \cdot \nabla_{x_n} \cdot \left( b_n^2 \psi \mathbf{I} \right) d\Gamma. \]
and has the form
\[
\int_{\Gamma} \left( \sum_{k=1}^{N} \Pi_k \right) \nabla_{x_n}^2 : \left( b_n^2 \psi I \right) d\Gamma =
\]
\[
= - \int_{\Gamma} \nabla_{x_n} \left[ \nabla_{x_n} \left( \sum_{k=1}^{N} \Pi_k \right) \cdot \left( b_n^2 \psi I \right) \right] d\Gamma +
\]
\[
+ \int_{\Gamma} \nabla_{x_n}^2 \left( \sum_{k=1}^{N} \Pi_k \right) : \left( b_n^2 \psi I \right) d\Gamma =
\]
\[
= \int_{\Gamma} \nabla_{x_n}^2 \left( \sum_{k=1}^{N} \Pi_k \right) : \left( b_n^2 \psi I \right) d\Gamma.
\]

With these identities, equality (6) becomes
\[
\int_{\Gamma} \frac{\partial}{\partial t} \left[ \left( \sum_{k=1}^{N} \Pi_k \right) \psi \right] d\Gamma - \int_{\Gamma} \sum_{n=1}^{N} \nabla_{x_n} \left( \sum_{k=1}^{N} \Pi_k \right) \cdot \left( \psi \mathbf{v}_n \right) d\Gamma -
\]
\[
- \frac{1}{2} \int_{\Gamma} \sum_{n=1}^{N} \nabla_{x_n}^2 \left( \sum_{k=1}^{N} \Pi_k \right) : \left( b_n^2 \psi I \right) d\Gamma = 0.
\]

The replacement of the operator \( \nabla_{x_n} \) by the operator \( -\nabla \) for the function \( \Pi_n \)
\[
\nabla_{x_n} \left( \sum_{k=1}^{N} \Pi_k \right) = \nabla_{x_n} \Pi_n = -\nabla \Pi_n,
\]
gives
\[
\int_{\Gamma} \frac{\partial}{\partial t} \left[ \left( \sum_{n=1}^{N} \Pi_n \right) \psi \right] d\Gamma + \int_{\Gamma} \sum_{n=1}^{N} \nabla \Pi_n \cdot \left( \psi \mathbf{v}_n \right) d\Gamma -
\]
\[
- \frac{1}{2} \int_{\Gamma} \sum_{n=1}^{N} \nabla^2 \Pi_n : \left( b_n^2 \psi I \right) d\Gamma = 0.
\]

where
\[
\nabla \ldots = \sum_{i=1}^{3} \mathbf{i}_i \frac{\partial}{\partial x^i} \ldots, \quad \nabla^2 \ldots = \nabla \left( \nabla \ldots \right).
\]

Taking the operations \( \partial/\partial t \) and \( \nabla \) out of the integration sign, we obtain the expression in question
\[
\frac{\partial}{\partial t} \int_{\Gamma} \sum_{n=1}^{N} \Pi_n \psi d\Gamma + \nabla \cdot \int_{\Gamma} \sum_{n=1}^{N} \Pi_n \psi \mathbf{v}_n d\Gamma -
\]
\[-\frac{1}{2} \nabla^2 : \int_{\Gamma} \sum_{n=1}^{N} I_n \, b_n^2 \psi \, I \, d\Gamma = 0. \]  

(6)

It can be used to derive the sufficient condition for transition to modeling the mass transfer based on the diffusion equation of the medium constituent.

### 5 Sufficient conditions for transition to continuum notions

The diffusion process can not be modeled using the notion of the chemical potential in the framework of the proposed approach. Such modeling must be based on the analysis of the first and second thermodynamic laws, the accounting of the interaction forces between the particles in the formulation of constitutive equations, and so on. With stochastic equations (1), the transition is possible to the Fick diffusion law only.

Define the notion of a diffusion coefficient \( D \) by the equality

\[ \rho D = \frac{m}{2} \int_{\Gamma} \sum_{n=1}^{N} I_n \, b_n^2 \psi \, d\Gamma. \]

To describe the process on the meso-level, it is sufficient to satisfy two conditions: the vectors \( v_n \) must obey the equality

\[ \rho v + \rho \nabla D = m \int_{\Gamma} \sum_{n=1}^{N} I_n \, v_n \, \psi \, d\Gamma, \]  

(7)

where \( v \) is the center-of-mass velocity of the body and the functional relation must exist between two values \( \rho \) and \( D \)

\[ D = D(\rho). \]  

(8)

With these requirements satisfied, equation (3) can be written in the form

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = \nabla \cdot (D \nabla \rho). \]

which is a well-known Fick law. The possibility to describe the process by the equation of continuous medium is checked, in particular problems, by conditions (1) and (8). It should be noted that we are dealing not with the averaged values, but with their mathematical expectations. In practice it means that these values should be calculated by averaging over space and random realizations.
6 Integral operator kernel of third order accuracy of image reproducing

For problem solution we should define a particular form of the integral operator kernel $\Pi$. We take the distance $r$ between the radius-vectors $\mathbf{x}$ and $\mathbf{x}_*$ as an argument of function $\Pi$

\[ \Pi = \Pi(r), \quad r = \sqrt{(\mathbf{x} - \mathbf{x}_*) \cdot (\mathbf{x} - \mathbf{x}_*)}. \]

To reproduce the effective density of particles most precisely, it is reasonable to use the function $\Pi(r)$ based on the ideas of constructing the integral operator kernel described by the RKPM method [5], [6].

The kernel $\Pi$ is supposed to meet the following requirements. Let some function $\beta(x)$ be represented as the coordinate dependence of the third order and the fast oscillating term $\gamma(x)$

\[ \beta(x) = b + b \cdot x + B : x \otimes x + 3 B : x \otimes x \otimes x + \gamma(x), \]

where $b$, $b$, $B$, $\gamma$ are tensors of zero, first, second and third rank. The cubic dependence must remain unchanged for any space point $x_*$ under the transition to the image performed by the integral operator

\[ \int_V \Pi(r) \left( b + b \cdot x + B : x \otimes x + 3 B : x \otimes x \otimes x \right) dV = b + b \cdot x_* + B : x_* \otimes x_* + 3 B : x_* \otimes x_* \otimes x_* . \]

The symbol $V$ stands for the entire volume of the Euclidean space. In the problems where the fast pulsations of the function $\gamma(x)$ suppress each other under integral transformation, i.e.,

\[ \int_V \Pi(r) \gamma(x) dV \approx 0, \]

the smoothed integral image of the initial function $\beta(x)$ will be the slowly changing cubic function

\[ \int_V \Pi(r) \beta(x) dV \approx b + b \cdot x_* + B : x_* \otimes x_* + 3 B : x_* \otimes x_* \otimes x_* . \]

In this case the integral operator will work as a "filter" that keeps slowly changing regularities and cancels fast pulsations.

Determine the conditions which the integral operator of the third order accuracy should satisfy. The function $\beta(x)$ may be developed as a series in powers
of \( \Delta x \) about point \( x \)

\[
\beta(x) = b + b \cdot x + B : x \otimes x + \frac{3}{3} B : x \otimes x \otimes x +
+ a + a \cdot \Delta x + A : \Delta x \otimes \Delta x + \frac{3}{3} A : \Delta x \otimes \Delta x \otimes \Delta x + \gamma(x),
\]

where

\[
\Delta x = x - x_* = \Delta x^1 i_1 + \Delta x^2 i_2 + \Delta x^3 i_3,
\]

\( a, a, A, A \) are tensors of zero, first, second and third rank. We note that equality (9) will be true only when the reproducing conditions are fulfilled

\[
\int_V \Pi(r) dV = 1, \quad \int_V \Pi(r) \Delta x dV = 0, \quad \int_V \Pi(r) \Delta x \otimes \Delta x dV = 0, \quad \int_V \Pi(r) \Delta x \otimes \Delta x \otimes \Delta x dV = 0.
\]

It is easy to find that in the spherical system of coordinates

\[
\Delta x^1 = r \cos(\alpha) \sin(\theta),
\]

\[
\Delta x^2 = r \sin(\alpha) \sin(\theta),
\]

\[
\Delta x^3 = r \cos(\theta)
\]

the reproducing conditions (10), (11) are equivalent to the requirement that the following equalities are valid

\[
\int_0^a r^2 \Pi(r) dr = \frac{1}{4\pi}, \quad \int_0^a r^4 \Pi(r) dr = 0.
\]

An example of the operator kernel of third order accuracy is the function

\[
\Pi(r) = \frac{1}{a_r^2} \left( \gamma_0 + \gamma_1 \frac{r^2}{a_r^2} \right) \left( 1 - \frac{r^2}{a_r^2} \right)^2 H(a_r - r)
\]

in which the constants \( \gamma_0, \gamma_1 \) are chosen such that equations (10), (11) are satisfied and the symbol \( H(...) \) denotes the Heaviside function.

7 Integral operator kernel of first order accuracy of image reproducing

The transition from physical to structural level may be performed using integral operators of first order accuracy. These operators must meet the requirement that only linear dependences retain in integral transformation

\[
\int_V \Pi(r) \left( b + b \cdot x \right) dV = b + b \cdot x_*.
\]
An example of integral operator kernels of first order accuracy is the function

\[
\Pi(r) = \frac{\gamma}{a_r^3} \left(1 - \frac{r^2}{a_r^2}\right)^2 H(a_r - r)
\]

and

\[
\Pi = \begin{cases} 
\frac{\gamma}{a_r}, & 0 \leq r < a_r; \\
\frac{\gamma}{2a_r^2} \left(1 + \cos \left(\pi \frac{r - a_r}{a_r - a_\gamma}\right)\right), & a_\gamma \leq r < a_r; \\
0, & a_r \leq r,
\end{cases}
\]  

(12)

in which constants \(\gamma\) are determined from the normalization condition

\[
\int_0^{a_r} r^2 \Pi(r) \, dr = \frac{1}{4\pi}.
\]

8 Numerical experiments

In this section, we consider the problem of penetration of diffusing particles into a semi-infinite material with constant concentration of particles on the material boundary. The constant \(b\) will be used as a function \(b_n\)

\[
b_n = b, \quad n = 1, \ldots, N,
\]

and all vectors \(v\) and \(v_n\) are assumed to be zero

\[
v = 0, \quad v_n = 0, \quad n = 1, \ldots, N.
\]

In this case, equations (7) and (8) are valid. The diffusion coefficient is found by the formula

\[
D = \frac{b^2}{2}.
\]

The performed numerical experiments demonstrated that the best smoothing effect can be achieved with the aid of the function \(\Pi(r)\) of first order accuracy of image reproducing (12). This function must be constant in the region occupying the half of the spherical volume of radius \(a_r\). In the present work, graphs (Fig. 1, Fig. 2) have been plotted based on the relation (12).

The obtained numerical results led us to the conclusion that the analytical solution of the Fick equation [7] is in good agreement with the fluctuating density \(\tilde{\rho}\) only in the case of a great number of particles in the averaging region. For example, about 5000 particles entered the radius sphere \(a_r\) on the material boundary when we calculated the dependence shown in Fig. 1.a.

An essential divergence between the fluctuating density \(\tilde{\rho}\) and the analytical solution can be observed under random realization of the process, in the course
Figure 1: Comparison of the theoretical diffusive profile with the numerical results when the concentration of diffusing particles on the material boundary is (a) 5000 per unit volume and (b) 30 per unit volume.
Figure 2: Comparison of the theoretical diffusive profile with the numerical results when the concentration of diffusing particles on the material boundary is 30 per unit volume. The results were averaged over 30 random realizations of which 30 particles enter the sphere with radius $a_r$ on the material boundary (Fig. 1b). However, one can also obtain the mesolevel images of the process. For this, it is sufficient to perform the averaging of the fluctuating density over thirty random realizations. The obtained density $\langle \rho \rangle$ agrees fairly well with the analytical solution of the Fick equation (Fig. 2) and is close to its most probable value (mathematical expectation, i. e. the density $\rho$).

9 Conclusion

The state parameters for the medium studied (mass density, diffusion coefficients) can be calculated with the aid of operators acting on a multitude of microscopic parameters $a_1, \ldots, a_N$ and having the form

$$L_1(a_1, \ldots, a_N) = \sum_{n=1}^{N} \Pi_n a_n.$$ 

and

$$L_2(a_1, \ldots, a_N) = \int \sum_{n=1}^{N} \Pi_n a_n \psi d\Gamma,$$

where $a_n$ is the characteristic of the $n^{th}$ particle. The fist operator represents the averaging procedure in the vicinity of the considered point in the Euclidean space.
and leads to the fluctuating twice differentiated variables. The second operator gives the determinate continuous twice-differentiated parameters, which can be used as the state characteristics of a continuous medium. Determination of diffusive profiles analogous to those on the mesolevel based on the fluctuating mass density is possible provided that thousands of particles enter the region of averaging. However, there is another way of constructing the mesolevel images of the process. It consists in averaging over the fluctuating densities calculated in numerical experiments. The results achieved in this case agree fairly well with the calculation data obtained on the level of continuous medium with much smaller number of particles entering the averaging region.

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