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Statistical modelling of mass transfer in turbulent twophase dispersed flows — 1. Model development

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Abstract

A closed equation for probability density function (PDF) of particles coordinates and velocities in a nonhomogeneous turbulent flow is obtained. On the base of the equation for PDF, a closed system of balance equations for concentration, momentum and energy of a chaotic motion of dispersed phase in Eulerian variables is derived. For the system of balance equations boundary conditions, describing particles interaction with a surface in a two-phase flow are found. © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

Turbulent liquid or gas flows with dispersed phase of particles or drops are widely used in power plants and chemical engineering equipments. In designing systems of pneumatic and hydro-transport of dispersed materials, it is necessary to predict the particles deposition rate on channel walls. The movement of particles to the walls in a turbulent flow can be induced by forces that are not directly associated with the flow regime, such as, forces of gravity, electrical field and thermophoresis. On the other hand, there are the mechanisms of a pure turbulent nature that cause particles deposition on the channel walls in the absence of external forces applied to the particles. The intensity of turbulent mass transfer of dispersed phase depends on the particles involving in a chaotic motion of the continuous medium. The rate of mass transfer due to nonhomogeneity of the turbulent flow parameters in the channel may be considerably higher than the rate of mass transfer under the action of external forces. In

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this case, we deal with purely turbulent mass transfer, ignoring any additional forces acting on particles.

The review of semi-empirical methods for calculating turbulent transport of dispersed particles was observed, for example, in Ganic and Mastanaiah [1] and Papavergos and Hedley [2]. However, the area of applicability of these semi-empirical relations is limited by a narrow class of flows. An approximate model of near-wall turbulent vortices was utilized in Fichman [3] and Fan and Ahmady [4] to estimate the intensity of particles turbulent deposition. The mass transfer models presented in Gusev et al. [5] and Swailes and Reeks [6] were based on the concept of an inertial flight of particles near the channel walls. The advent of powerful high-speed computers makes it possible to carry out direct numerical simulations (DNS) of the statistical characteristics of the continuum phase and the random Lagrangian trajectories of the particles, for example, Uijttewaal and Oliemans [7], Soltani et al. [8], Simonen et al. [9]. However, DNS methods are generally limited to the low Reynolds number cases. Furthermore, the run of these methods for two-phase turbulent dispersed flows requires tens of hours

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Nomenclature

С	volume concentration of dispersed phase
$C_{ m m}$	mean volume concentration of dispersed
	phase
D_{ij}^{p}	coefficient of particles turbulent diffu-
J	$\sin (m^2 s^{-1})$
D^{o}_{ii}	coefficient of turbulent diffusion of pas-
	sive impurity $(m^2 s^{-1})$
E_{ij}	Eulerian correlation of fluid velocity
	fluctuations (m ² s ^{-2})
F	fluxes of dispersed phase parameters
g_i	acceleration of mass force (m s^{-2})
g_p, h_p	response function of particles
J	velocity of particles deposition on a sur-
	face (m s ⁻¹)
k_n, k_t	coefficients of impulse restitution in nor-
	mal and axial directions
$\hat{L}_{\rm E}$	Eulerian integral length scale (m)
	operator in Eq. (35)
L_p	parameters of dispersed phase (m)
T	parameters of dispersed phase (iii)
L_0	phase flow (m)
1	distance of a particle inertial flight (m)
$\frac{l_p}{N}$	number of particles in the volume Q ₁
n a	number of particles in the volume M_N
P_p, q_p R_n	position of <i>p</i> th particle (m)
r_p	fluctuations of a particle position (m)
$T_{\rm E}, T_{\rm I}$	Eulerian and Lagragian time scales (s)
T_n^{L}	integral time scale of fluid velocity fluc-
P	tuations along a particle path (s)
U	actual velocity of fluid phase (m s^{-1})
и	fluid velocity fluctuations (m s^{-1})
V	actual velocity of dispersed phase (m
	s^{-1})
V_p	actual velocity of <i>p</i> th particle (m s ^{-1})
V', V''	particle velocity before and after col-
	lision with a wall (m s^{-1})
\boldsymbol{v}_p	velocity fluctuation of pth particle (m
	s^{-1})
W	averaged relative velocity of dispersed
	phase (m s^{-1})

x, y, z Ca	artesian	coordinate	system	(m))
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- Z_p probability density function of a particle transition
- *Z*_W transformation function of particles velocity during wall collisions

Greek symbols

a a	parameter characterizes the "crossing
	trajectory effect", W/u
β	ratio of Lagrangian and Eulerian inte-
	gral time scales of turbulence, $T_{\rm L}/T_{\rm E}$
γ	parameter coupled with internal struc-
·	ture of turbulence, $uT_{\rm L}/L_{\rm E}$
Δ	Heaviside step-function
δ	Dirac delta-function
δ_{ij}	Kronecker delta
Σ	turbulent stresses in dispersed phase (m ²
	s^{-2})
$\sigma_{ij} = \langle v_i v_j \rangle$	the correlation between components of
	the dispersed phase turbulent velocity
	$(m^2 s^{-2})$
$ au_p$	dynamic relaxation time of <i>p</i> th particle
	(s)
ω_p	volume of p th particle (m ³)
Φ, φ	PDF particles velocities and coordinates
	and PDF only particles velocities, re-
	spectively
χ	absorption coefficient
${\Psi}_{ m E}$	Eulerian autocorrelation function of
	fluid phase velocity fluctuations
Ψ_p	fluid velocity autocorrelation function
0	along a particle trajectory
$\Omega_{\rm E}$	parameter of p articles inertia, τ_p/I_E
Ω_N	volume of a now with N particles (m)
Subscripts	
n	denotes parameters belonging to <i>p</i> th
Ľ	particle
+	denote parameters of dropping and
7	reflecting particles

processor time on superpowerful computers, that limits the applicability area of these methods to purely theoretical problems.

For practical purposes, the most effective method for calculating turbulent two-phase flows is based on equations written in Eulerian variables. In this case, turbulence of dispersed impurity is described within the framework of the equations, similar to the equations of continuous medium. This allows to use huge experience that was accumulated in calculating single-phase turbulent flows. The method based on the PDF approach for particles characteristics was employed in Reeks [10] and Derevich [11] for transition from Lagrangian equations of an individual particle motion and interaction of the particle with a surface to the system of balance equations for dispersed phase in Eulerian variables. The equations for PDF of particles are comparable with the Fokker– Planck equation. Equation for particles diffusion in a random velocity field and boundary condition takes into account the particles interaction with absorbing/reflected walls, which was directly designed from the Fokker–Planck equation by Nagvi et al. [12], Protopopescu and Keyes [13] and Menon et al. [14]. The designed boundary condition represents association between a gradient of particles concentration and the particles concentration on the wall and involves an absorption coefficient.

A different technique for derivation the closed system of equation for hydrodynamics and mass transfer of dispersed phase with complemented boundary conditions was proposed by Derevich and Yeroshenko [15]. The boundary conditions take into account an exchange of impulse and heat between particles and wall. The mathematical procedure used in [15] was based on the approximate solution of the closed PDF equation. This procedure is linked with the Chapman– Enskog method in the kinetic theory of gases.

This study is devoted to the generalization of PDF approach to describe turbulent two-phase flow with dispersed phase in Eulerian variables. We achieved the closed equation for particles PDF in nonhomogeneous and nonstationary turbulent flow. On the basis of approximate solution of the PDF equation, we discovered a closed system of balance equations for concentration, momentum and turbulent energy of dispersed phase. Complemented boundary conditions with regard to the particles absorption and loss of particles impulse after collision with a surface are also determined.

2. Equation for PDF

2.1. Average and fluctuating quantities

Particles of the spherical form are considered, size of which is less then Kolmogorov turbulent spatial microscale. In this case, dispersed particles may be modeled as mathematical points. Similar situation is realized, as a rule, at turbulent flow of gas with particles or droplets. Particles concentration is sufficiently diluted such that any particle–particle collisions can be ignored. In the Lagrangian equations for individual particle motion in continuous medium, we take into account only the viscous drag and gravitational forces

$$\frac{\mathrm{d}V_{pi}(t)}{\mathrm{d}t} = \frac{1}{\tau_p} \left(U_i(\boldsymbol{R}_p, t) + \tau_p g_i - V_{pi} \right),$$

$$\frac{\mathrm{d}R_{pi}(t)}{\mathrm{d}t} = V_{pi}$$
(1)

where $U_i(\mathbf{x}, t)$ is the velocity of a liquid phase, $\mathbf{R}_p(t)$,

 $V_p(t)$ are the position and velocity of a *p*th particle, and τ_p is the *p*th particle dynamic relaxation time, which is dependent on particle relative velocity, g_i is the gravitational acceleration.

For passing from Lagrangian variables in Eq. (1) to Eulerian variables, we determine instantaneous PDF of particles coordinates and velocities

$$\Phi(\mathbf{x}, \mathbf{V}, t) = \sum_{p=1}^{N} \frac{\omega_p}{\Omega_N} \delta(\mathbf{x} - \mathbf{R}_p) \delta(\mathbf{V} - \mathbf{V}_p)$$
(2)

where ω_p is the volume of the *p*th particle, Ω_N the volume of flow, containing N particles, and $\delta(\mathbf{x})$ the Dirac delta function.

Volumetric concentration and velocity of dispersed phase are expressed through the PDF

$$C(\mathbf{x}, t) = \sum_{p=1}^{N} \frac{\omega_p}{\Omega_N} \delta(\mathbf{x} - \mathbf{R}_p) = \int \Phi \, \mathrm{d}\mathbf{V}$$
(3)

$$C(\mathbf{x}, t)V(\mathbf{x}, t) = \sum_{p=1}^{N} \frac{\omega_p}{\Omega_N} V_p \delta(\mathbf{x} - \mathbf{R}_p) = \int V \Phi \, \mathrm{d}V \qquad (4)$$

After averaging over an ensemble of turbulent realizations from definitions (2)–(4), we carry out the average PDF, concentration, and average velocity of the dispersed phase

$$\langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle = \left\langle \sum_{p=1}^{N} \frac{\omega_p}{\Omega_N} \delta(\mathbf{x} - \mathbf{R}_p) \delta(\mathbf{V} - \mathbf{V}_p) \right\rangle$$
$$\langle C(\mathbf{x}, t) \rangle = \left\langle \sum_{p=1}^{N} \frac{\omega_p}{\Omega_N} \delta(\mathbf{x} - \mathbf{R}_p) \right\rangle = \int d\mathbf{V} \langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle \quad (5)$$

$$\langle C(\mathbf{x}, t) \rangle \langle V(\mathbf{x}, t) \rangle = \left\langle \sum_{p=1}^{N} \frac{\omega_p}{\Omega_N} V_p \delta(\mathbf{x} - \mathbf{R}_p) \right\rangle$$
$$= \int V \langle \Phi \rangle \, \mathrm{d}V \tag{6}$$

The instantaneous particle velocity we combine as the sum of the averaged dispersed phase velocity at the point $\mathbf{x} = \mathbf{R}_{p}(t)$ and the fluctuating component

$$\boldsymbol{V}_{p}(t) = \langle \boldsymbol{V}(\boldsymbol{x}, t) \rangle + \boldsymbol{v}_{p}(t) = \langle \boldsymbol{V}(\boldsymbol{R}_{p}(t), t) \rangle + \boldsymbol{v}_{p}(t)$$
(7)

By analogous expression (4) we define the fluctuating component of the dispersed phase velocity

$$C(\boldsymbol{x}, t)\boldsymbol{\nu}(\boldsymbol{x}, t) = \sum_{p=1}^{N} \frac{\omega_p}{\Omega_N} \boldsymbol{\nu}_p(t) \delta(\boldsymbol{x} - \boldsymbol{R}_p)$$
(8)

From relations (5)–(8), the value of correlation between concentration and velocity fluctuation of the dispersed phase is zero

$$\langle C \boldsymbol{v} \rangle = \left\langle \sum_{p=1}^{N} \frac{\omega_p}{\Omega_N} \boldsymbol{v}_p \delta \left(\boldsymbol{x} - \boldsymbol{R}_p \right) \right\rangle \equiv 0$$

The previous definition of fluctuating part of particles velocity corresponds well with the common definition of the fluctuating velocity component and PDF

$$\int (V - \langle V \rangle) \langle \Phi \rangle \, \mathrm{d}V = \int v \langle \Phi \rangle \, \mathrm{d}v = 0$$

We obtain from Eq. (7), the expression for the particle instantaneous displacement

$$\boldsymbol{R}_{p}(t) = \langle \boldsymbol{R}_{p}(t) \rangle + \boldsymbol{r}_{p}(t) = \int_{0}^{t} \boldsymbol{V}_{p}(s') \, \mathrm{d}s'$$
$$= \int_{0}^{t} [\langle \boldsymbol{V} \big(\boldsymbol{R}_{p}(s'), s' \big) \rangle + \boldsymbol{v}_{p}(s')] \, \mathrm{d}s'$$
(9)

2.2. Derivation of the PDF equation

In the terms of fluctuating velocity of dispersed phase, we write down the equation for averaged PDF $\langle \Phi(\mathbf{x}, \mathbf{v}, t) \rangle$

$$\frac{\partial \langle \Phi \rangle}{\partial t} + (\langle V_k \rangle + v_k) \frac{\partial \langle \Phi \rangle}{\partial x_k} - \left[\frac{\partial \langle V_i \rangle}{\partial t} + (\langle V_k \rangle + v_k) \frac{\partial \langle V_i \rangle}{\partial x_k} - \frac{1}{\tau_p} (\langle U_i \rangle + \tau_p g_i - \langle V_i \rangle) \right] \frac{\partial \langle \Phi \rangle}{\partial v_i} = -\frac{\partial}{\partial v_i} \frac{1}{\tau_p} (\langle u_i \Phi \rangle - v_i \langle \Phi \rangle)$$
(10)

For obtaining the closed form of the Eq. (10), it is necessary to find an expression for correlation between turbulent velocity of continuous phase and PDF $\langle u\Phi \rangle$. We approximate turbulent velocity fluctuation of carrying phase by a random Gaussian field [16]. This assumption is acceptable for energetic turbulent eddies. We investigate the response of particles on the energetic turbulent eddies. In this case, presentation of fluid turbulent velocity as the normal Gaussian process is satisfactory. Based on this assumption, with the assistance of the method of functional derivative, we write the Furutsu–Novikov (Klyatskin [17]) expression for correlation between turbulent fluid velocity and PDF in Eq. (10)

$$\langle u_i \Phi \rangle = \int_0^t \, \mathrm{d}\xi \int \, \mathrm{d}\mathbf{x}_1 \langle u_i(\mathbf{x}, t) u_j(\mathbf{x}_1, \xi) \rangle \langle \frac{\delta \Phi(\mathbf{x}, \mathbf{v}, t)}{\delta u_j(\mathbf{x}_1, \xi)} \rangle \tag{11}$$

Here, the functional derivative from PDF becomes

$$\frac{\delta \Phi(\mathbf{x}, \mathbf{v}, t)}{\delta u_j(\mathbf{x}_1, \xi)} = -\frac{\partial}{\partial x_k} \Phi \frac{\delta R_{pk}(t)}{\delta u_j(\mathbf{x}_1, \xi)} - \frac{\partial}{\partial v_k} \Phi \frac{\delta v_{pk}(t)}{\delta u_j(\mathbf{x}_1, \xi)} \quad (12)$$

Functional derivative from particles position is determined considering definition (9)

$$\frac{\delta R_{pj}(t)}{\delta u_k(\mathbf{x}_1, s)} = \frac{\partial \langle V_j \rangle}{\partial x_n} \int_0^t \frac{\delta r_{pn}(s')}{\delta u_k(\mathbf{x}_1, s)} ds' + \int_0^t \frac{\delta v_{pj}(s')}{\delta u_k(\mathbf{x}_1, s)} ds'$$
(13)

In the functional derivation $\delta R_{pj}/\delta u_k$, we take into account only part $\delta r_{pj}/\delta u_k$, because dependence of the average part $\langle R_{pj}(t) \rangle$ on the turbulent fluid velocity is not so strong as particle fluctuation displacement $r_{pj}(t)$.

To derive of the equation for chaotic particle velocity in nonhomogeneous turbulent flow, we utilize the definition of particles fluctuating velocity (7). In conformity with relations (1) and (7) we write the equation

$$\begin{aligned} \frac{\mathrm{d} V_{pj}}{\mathrm{d} t} &= \frac{1}{\tau_p} \Big[U_j \big(\boldsymbol{R}_p(t), t \big) - V_{pj}(t) \Big] \\ &= \frac{1}{\tau_p} \Big[\langle U_j \rangle - \langle V_j \rangle + u_j - v_{pj} \Big] \\ &= \frac{\mathrm{d} v_{pj}(t)}{\mathrm{d} t} + \frac{\partial \langle V_j(\boldsymbol{x}, t) \rangle}{\partial t} |_{\boldsymbol{x} = \boldsymbol{R}_p} \\ &+ V_{pk}(t) \frac{\partial \langle V_j(\boldsymbol{x}, t) \rangle}{\partial x_k} |_{\boldsymbol{x} = \boldsymbol{R}_p} \end{aligned}$$

We take into account only fluctuating members in this equation and thus obtain

$$\frac{\mathrm{d}v_{pj}(t)}{\mathrm{d}t} + v_{pk}(t) \frac{\partial \langle V_j(\boldsymbol{R}_p(t), t) \rangle}{\partial x_k}
= \frac{1}{\tau_p} \Big[u_j(\boldsymbol{R}_p(t), t) - v_{pj}(t) \Big]$$
(14)

We interpret Eq. (14) as an integral equation

$$v_{pj}(t) = \frac{1}{\tau_p} \int_0^t \exp\left(-\frac{t-s}{\tau_p}\right) \left[u_j(\boldsymbol{R}_p(s), s) - \tau_p v_{pk}(s) \frac{\partial \langle V_j(\boldsymbol{R}_p(s), s) \rangle}{\partial x_k} \right] ds$$
(15)

From Eq. (15) one can see that in a nonhomogeneous flow, random movement of inertial particles intensify the dispersed phase chaotic motion. Energy of particles chaotic motion is determined by a degree of particles entrainment in turbulent fluctuations of large powerful eddies of the carrying phase. We suppose, that the primary source of energy of particles chaotic motion coupled with turbulent velocity fluctuations of fluid phase, and take into account the gradient of averaged velocity of dispersed phase as the first correction. At this assumption, particles fluctuation velocity at the term with a gradient of averaged velocity in Eq. (15) is presented as

$$v_{pk}(s) = \frac{1}{\tau_p} \int_0^s \exp\left(-\frac{s-s'}{\tau_p}\right) u_j(\boldsymbol{R}_p(s'), s') \,\mathrm{d}s' \tag{16}$$

Within the framework of this approximation from Eqs. (15) and (16) we find the expression for chaotic velocity of particles in the nonhomogeneous turbulent flow

$$v_{pj}(t) = \int_{0}^{t} Au'_{j} \frac{\mathrm{d}s}{\tau_{p}} - \tau_{p} \frac{\partial \langle V_{j} \rangle}{\partial x_{k}} \int_{0}^{t} \left(\frac{t-s}{\tau_{p}}\right) Au'_{k} \frac{\mathrm{d}s}{\tau_{p}}$$

$$A = \exp\left(-\frac{t-s}{\tau_{p}}\right), \boldsymbol{u}' = \boldsymbol{u}\left(\boldsymbol{R}_{p}(s), s\right)$$
(17)

Introducing formula (17) into Eq. (9), we get the expression for the random displacement of the particle

$$r_{pj}(t) = \int_0^t (1-A)u_j' \,\mathrm{d}s - \tau_p^2 \frac{\partial \langle V_j \rangle}{\partial x_k} \int_0^t \left\{ (1-A) - \frac{(t-s)}{\tau_p} A \right\} u_k' \,\frac{\mathrm{d}s}{\tau_p}$$
(18)

Being restricted in Eqs. (16) and (17) by the first-order averaged velocity derivatives of the dispersed phase, we determine the functional derivations in Eqs. (11)and (12)

$$\frac{\delta v_{pj}(t)}{\delta u_k(\mathbf{x}_1, s)} = \delta(\mathbf{x}_1 - \mathbf{R}_p(s)) \left\{ \frac{\delta_{jk}}{\tau_p} A - \frac{\partial \langle V_j \rangle}{\partial x_k} \left(\frac{t-s}{\tau_p} \right) A \right\}$$
(19)

$$\frac{\delta R_{pj}(t)}{\delta u_k(\mathbf{x}_1, s)} = \delta(\mathbf{x}_1 - \mathbf{R}_p(s)) \left\{ \delta_{jk}(1 - A) + \tau_p \frac{\partial \langle V_j \rangle}{\partial x_k} \left[\frac{(t - s)}{\tau_p} (1 + A) - 2(1 - A) \right] \right\}$$
(20)

In Appendix A, a calculation technique with application of functional differentiation is submitted.

It is understood from Eqs. (10), (11), (19) and (20) that expression for the correlation $\langle u_i \Phi \rangle$ includes corre-

lation of fluid velocity fluctuations along the particle trajectory. This correlation may be expressed in the following form

$$\langle u_i(\boldsymbol{x}, t)u_j(\boldsymbol{R}_p(s), s)\rangle = \langle u_i(\boldsymbol{x}, t)u_j(\boldsymbol{x} - \boldsymbol{R}_p(\boldsymbol{\xi}), t - \boldsymbol{\xi})\rangle \quad (21)$$

where

$$\xi = t - s$$
, and $\boldsymbol{R}_p(t) = \boldsymbol{x}$.

2.3. Fluid phase velocity correlation along the particle trajectory and particles response functions

The fluid velocity correlation (21) depends on macroscales, which are proportional to the size of variation area of the averaged flow parameters, and microscales joined with internal microstructure of turbulence

$$\langle u_i(\mathbf{x}, t)u_j(\mathbf{x} - \mathbf{R}_p(\xi), t - \xi) \rangle$$

= $\langle E_{ij}(\mathbf{x} - 0.5\mathbf{R}_p(\xi), t - 0.5\xi; \mathbf{R}_p(\xi), \xi) \rangle$ (22)

Here E_{ij} is two-points and two-times Eulerian fluid velocity correlation in the coordinate system moving with averaged velocity of the fluid stream

$$E_{ij}(\mathbf{x}_{\alpha\beta}, t_{\alpha\beta}; \mathbf{Y}, \xi) = \langle u_i(\mathbf{x}_{\alpha}, t_{\alpha})u_j(\mathbf{x}_{\beta}, t_{\beta}) \rangle$$

$$t_{\alpha\beta} = 0.5(t_{\alpha} + t_{\beta}), \mathbf{x}_{\alpha\beta} = 0.5(\mathbf{x}_{\alpha} + \mathbf{x}_{\beta}), \mathbf{Y}$$

$$= \mathbf{x}_{\alpha} - \mathbf{x}_{\beta}$$
(23)

The averaging in correlation (22) is carried out over an ensemble of turbulent realizations, and random particles trajectories. Accepting significant differences between the value of scales of average variables $x_{\alpha\beta}$ (macroscales) and relative variables *Y* (internal turbulent scales) in expressions (22) and (23), we write down the series

$$\langle E_{ij} \left(\mathbf{x} - 0, 5\mathbf{R}_{p}(\xi), t - 0, 5\xi; \mathbf{R}_{p}(\xi), \xi \right) \rangle \approx \langle E_{ij} \rangle$$

$$- \frac{\xi}{2} \left\{ \frac{\partial}{\partial t} \langle E_{ij} \rangle + \langle \left(\langle V_{k} \rangle + v_{pk}(\xi) \right) \frac{\partial E_{ij}}{\partial x_{k}} \rangle \right\}$$

$$\langle E_{ij} \rangle = \langle E_{ij} \left(\mathbf{x}, t; \mathbf{R}_{p}(\xi), \xi \right) \rangle$$

$$(24)$$

After substitution of expressions (19), (20) and (24) in Eqs. (11) and (12), we obtain the particles response function, describing entrainment of dispersed phase in turbulent fluctuation of the carrying phase

$$\int_{0}^{t} A \langle E_{ij} \rangle \frac{d\xi}{\tau_{p}} = q_{p} \langle u_{i} u_{j} \rangle,$$

$$\int_{0}^{t} \frac{\xi}{\tau_{p}} A \langle E_{ij} \rangle \frac{d\xi}{\tau_{p}} = p_{p} \langle u_{i} u_{j} \rangle$$

$$\int_{0}^{t} \left\{ \frac{\xi}{\tau_{p}} (1+A) - 2(1-A) \right\} \langle E_{ij} \rangle \frac{d\xi}{\tau_{p}} = h_{p} \langle u_{i} u_{j} \rangle$$

$$\int_{0}^{t} (1-A) \langle E_{ij} \rangle \frac{d\xi}{\tau_{p}} = g_{p} \langle u_{i} u_{j} \rangle, \quad A = \exp\left(-\frac{\xi}{\tau_{p}}\right)$$
(25)

The function h_p is similar to that received earlier by Zaichik [18]. In the formulas (25), characteristic temporary scale of fluid phase velocity fluctuation along the particle trajectory is of the order of Eulerian integral time scale T_E . It should be pointed out that fluid velocity correlation (23) must satisfy the conditions of equilibrium (stationary conditions) at the turbulent internal microscales

$$\frac{\partial E_{ij}(\boldsymbol{Y},\,\boldsymbol{\xi})}{\partial \boldsymbol{\xi}} = \frac{\partial E_{ij}(\boldsymbol{Y},\,\boldsymbol{\xi})}{\partial Y_k} = 0, \quad \text{for } \boldsymbol{\xi} = 0 \text{ or } \boldsymbol{Y} = 0$$

For the inertial particle $\tau_p \gg T_{\rm E}$ from formulas (25) it follows that

$$q_p \propto T_{\rm E}/\tau_p, \quad p_p \propto g_p \propto \left(T_{\rm E}/\tau_p\right)^2, \quad h_p \propto \left(T_{\rm E}/\tau_p\right)^4$$
(26)

In a case of the particle with small inertia $\tau_p \ll T_{\rm E}$, we have

$$q_p \rightarrow p_p \rightarrow 1, \quad g_p \propto T_{\rm E}/\tau_p, \quad h_p \propto \left(T_{\rm E}/\tau_p\right)^2$$
 (27)

As a result of substitution Eqs. (19), (20) and (24) into Eqs. (11), we find an expression for the correlation $\langle u_i \Phi \rangle$, which produce the closed form for the PDF equation (10)

$$\langle u_i \Phi \rangle = -\tau_p G_p \langle u_i u_j \rangle \frac{\partial \langle \Phi \rangle}{\partial x_j} - Q_p \langle u_i u_j \rangle \frac{\partial \langle \Phi \rangle}{\partial v_j}$$
(28)

$$G_{p}\langle u_{i}u_{j}\rangle = g_{p}\langle u_{i}u_{j}\rangle + \frac{1}{2}\tau_{p}h_{p}\left(\langle u_{i}u_{k}\rangle\frac{\partial\langle V_{j}\rangle}{\partial x_{k}} + \langle u_{j}u_{k}\rangle\frac{\partial\langle V_{i}\rangle}{\partial x_{k}}\right)$$
(29)

$$Q_{p}\langle u_{i}u_{j}\rangle = q_{p}\langle u_{i}u_{j}\rangle - \frac{1}{2}\tau_{p}p_{p}\left[\frac{\partial\langle u_{i}u_{j}\rangle}{\partial t} + \langle V_{k}\rangle\frac{\partial\langle u_{i}u_{j}\rangle}{\partial x_{k}} + \frac{\partial\langle u_{i}u_{j}u_{k}\rangle}{\partial x_{k}} + \langle u_{i}u_{k}\rangle\frac{\partial\langle V_{j}\rangle}{\partial x_{k}} + \langle u_{j}u_{k}\rangle\frac{\partial\langle V_{i}\rangle}{\partial x_{k}}\right]$$
(30)

The expressions (29) and (30) include fluid velocity

correlation, terms connected with the gradient of the averaged velocity of the dispersed phase, and also terms representing nonstationary, convection and turbulent transfer of an intensity of chaotic motion. Without the account of the terms with the gradients of averaged dispersed phase parameters and nonstationary additives, the expressions (28)–(30) coincide with the appropriate expression obtained by Reeks [10].

In principle, PDF contains sufficient information about hydrodynamics turbulent parameters of the dispersed phase. However, it is very difficult to find an analytical or numerical solution of PDF equations (10) and (28) in a strongly nonhomogeneous turbulent flow, and we are forced to address the system of moment equations.

3. Equation for the first and second moments of dispersed phase velocity fluctuation

Out of the PDF equations (10) and (28), we can derive by the standard way the system equations for moment of dispersed phase velocity fluctuations.

The equations for concentration and averaged velocity of the dispersed phase look like

$$\frac{\partial \langle C \rangle}{\partial t} + \frac{\partial}{\partial x_i} \langle C \rangle \langle V_i \rangle = 0 \tag{31}$$

$$\frac{\partial \langle V_i \rangle}{\partial t} + \langle V_k \rangle \frac{\partial \langle V_i \rangle}{\partial x_k} + \frac{\partial \langle v_i v_k \rangle}{\partial x_k}$$
$$= \frac{\langle U_i \rangle + \tau_p g_i - \langle V_i \rangle}{\tau_p} - \frac{D_{ik}^p}{\tau_p} \frac{\partial \ln \langle C \rangle}{\partial x_k}$$
(32)

$$D_{ik}^{\mathbf{p}} = \tau_p \big(\langle v_i v_k \rangle + G_p \langle u_i u_k \rangle \big)$$
(33)

where D_{ik}^{p} is coefficient of particles turbulent diffusion.

The coefficient of turbulent diffusion Eq. (33) takes into account not only chaotic motion of particles (first term in right-hand side of (33)), but also dispersed phase turbulent motion with energy containing turbulent eddies (second term in the right-hand side of Eq. (33)). In the expression for turbulent diffusion of particles, enter gradients from the dispersed phase averaged velocity (expression (29)). Averaged velocity of dispersed phase is formed as a result of particles moving with the fluid velocity, action of the gravity force and collisions of particles with surface.

Second moments of velocity fluctuations in the lefthand side of Eq. (32) describe the turbulent stresses in the dispersed phase arising due to involvement of particles in turbulent motion.

In Eq. (32), we ignore the influence of the Saffman [19] lift force on the particles motion. This is due to

two reasons. First, the formula for this lift force was obtained by Saffman for steady-state laminar flow. Consequently, the accurate analysis is required to decide whether this expression can be applied to turbulent flow near the wall, where the level of fluctuations of the axial velocity is comparable in magnitude with the averaged velocity of the flow. Second, the results of DNS of two-phase dispersed flow, for example, Uijttewaal and Oliemans [7], indicate that turbulence and particles inertia dominate over the Saffman lift in the transport of dispersed impurity.

The equation for the second moments of dispersed phase velocity fluctuations also follows from the PDF equations (10) and (28)

$$\frac{\partial \langle v_{i}v_{j} \rangle}{\partial t} + \langle V_{k} \rangle \frac{\partial \langle v_{i}v_{j} \rangle}{\partial x_{k}} + \frac{1}{\langle C \rangle} \frac{\partial \langle C \rangle \langle v_{i}v_{j}v_{k} \rangle}{\partial x_{k}} + \langle v_{i}v_{k} \rangle \frac{\partial \langle V_{j} \rangle}{\partial x_{k}} + \langle v_{j}v_{k} \rangle \frac{\partial \langle V_{i} \rangle}{\partial x_{k}} = \frac{2}{\tau_{p}} (Q_{p} \langle u_{i}u_{j} \rangle - \langle v_{i}v_{j} \rangle) \langle v_{i}v_{j}v_{k} \rangle \langle C \rangle = \int v_{i}v_{j}v_{k} \langle \Phi \rangle d\mathbf{v}$$
(34)

Here, the third correlation of velocity fluctuation describes the turbulent transport of the energy of chaotic motion in the dispersed phase. The term with the second fluid velocity correlation in the right part of Eq. (34) expresses a source of the particles chaotic motion.

For particles with small inertia $\tau_p \ll T_E$ energy of a chaotic motion of the dispersed impurity and carrying phase are identical. From the behaviour of particles response functions (25) in the cases of inertial (26) and low inertial particles (27), it follows that in the source term of dispersed phase chaotic motion in Eq. (34), we can take into account only participation of particles in turbulent motion of energy containing eddies

 $Q_p \langle u_i u_j \rangle \approx q_p \langle u_i u_j \rangle$

4. Calculation of time scale of fluid velocity correlation along a particle path

The functions of particles reaction on turbulent velocity fluid fluctuations (25) are controlled by the relation between particles contact time with large turbulent eddies and particles relaxation time. The fluid velocity correlation in Eq. (25) associates with the coordinate system driven together with the carrying stream. We may write the expression for fluid velocity correlations along the particle path in the following form

$$\left\langle E_{ij}\left(\mathbf{x}, t; \mathbf{R}_{p}'(\xi), \xi\right) \right\rangle$$

$$= \int \langle E_{ij}\left(\mathbf{x}, t; \mathbf{Y}_{p}, \xi\right) Z_{p}\left(\mathbf{Y}_{p}, \xi\right) \rangle \, \mathrm{d}\mathbf{Y}_{p}$$

$$Z_{p}\left(\mathbf{Y}_{p}, \xi\right) = \delta\left(\mathbf{Y}_{p} - \mathbf{R}_{p}'(\xi)\right)$$

$$(35)$$

where $Z_p(Y_p, \xi)$ is a probability density function of the particle transition during time ξ for the distance Y_p ; $R'_p, V'_p = V_p - \langle U \rangle$ are the position and velocity of the particle in the coordinate system, respectively, moving with the fluid stream.

We approximate the change of the particle position during the time of life of turbulent energetic eddies by the expression

$$\boldsymbol{R}_{p}^{\prime}(\boldsymbol{\xi}) = \int_{0}^{\boldsymbol{\xi}} \boldsymbol{V}_{p}^{\prime}(\boldsymbol{\xi}^{\prime}) \boldsymbol{\xi}^{\prime} \approx (\boldsymbol{W} + \boldsymbol{\nu}) \boldsymbol{\xi},$$

$$\boldsymbol{W} = \langle \boldsymbol{V} \rangle - \langle \boldsymbol{U} \rangle$$
(36)

where W is averaged relative velocity slip between continuous and dispersed phases; v is the characteristic amplitude of particles velocity fluctuation.

For estimation of the dispersed phase velocity fluctuation ν in Eq. (36), we used the PDF in the local equilibrium assumption. We approximate the particles velocity fluctuation as the Gaussian random process, and from expressions (35) and (36) obtain presentation for fluid turbulent velocity correlation along the particle path

$$\left\langle E_{ij}(\mathbf{x}, t; \mathbf{R}'_{p}(\xi), \xi) \right\rangle \approx \int E_{ij}(\mathbf{x}, t; (\mathbf{W} + \mathbf{v})\xi, \xi) \varphi(\mathbf{v}) \, \mathrm{d}\mathbf{v}$$

$$(37)$$

$$\varphi(\mathbf{v}) = \prod_{i=1}^{3} \frac{1}{(2\pi\sigma_{ii})^{1/2}} \exp\left(-\frac{v_i^2}{2\sigma_{ii}}\right), \quad \sigma_{ij} = \langle v_i v_j \rangle \qquad (38)$$

where $\varphi(v)$ is the PDF of dispersed phase velocity fluctuations. This PDF can be found as the solution to PDF equation (10) for a stationary and homogeneous turbulent flow.

Integral time scale for correlation of fluid turbulent velocity along the particle trajectory is calculated considering expression (37)

$$T_{p}(\mathbf{x}, t) = \langle u_{i}u_{j}\rangle^{-1} \int d\mathbf{v} \int_{0}^{\infty} E_{ij}(\mathbf{x}, t; (\mathbf{W} + \mathbf{v})\xi, \xi) \varphi(\mathbf{v}) d\xi$$
(39)

The Eulerian turbulent fluid velocity correlation in Eq. (39) was chosen in the form

$$E_{ij}(\mathbf{x}, t; \mathbf{y}, \xi) = \langle u_i u_j \rangle \Psi_{\rm E}(\mathbf{y}, \xi),$$
$$\Psi_{\rm E}(\mathbf{y}, \xi) = \exp\left(-\frac{|\mathbf{y}|^2}{L} - \frac{\xi^2}{T}\right), \quad T_{\rm E} = \frac{\sqrt{\pi}}{2}T, \qquad (40)$$
$$L_{\rm E} = \frac{\sqrt{\pi}}{2}L$$

where $L_{\rm E}$ is Eulerian spatial integral macroscale in the moving coordinate system.

Particle contact time with turbulent eddies is similar to the integral time scale of the carrying phase velocity fluctuations along the particle trajectory. From Eqs. (39) and (40) we achieve the expression for the integral time scale

$$\frac{T_p}{T_E} = \frac{1}{A^3} \left[1 + \left(\frac{\gamma}{\beta}\right)^2 \left(\frac{\alpha}{A}\right)^2 \right]^{-1/2},$$

$$A = \left[1 + \frac{\pi}{2} q_p \left(\frac{T_p}{T_E}\right)^2 \left(\frac{\gamma}{\beta}\right)^2 \right]^{1/2}$$
(41)

where $\beta = T_L/T_E$ is the ratio of integral time scales of turbulence in Lagrangian T_L and Eulerian variables; parameter $\alpha = W/u$ describes the effect of "crossings trajectories" on the particles turbulent motion energy; parameter $\gamma = uT_L/L_E$ is coupled to internal turbulent microstructure and is determined by the type of flow (Krashenninnikov and Secundov [20]) and the flow Reynolds number Sato and Yamamoto [21]). In the Appendix B, a derivation and analysis of the formula (41) is submitted.

From expression (41) it follows that with growth of the relative velocity between the phases, contact time of particles with turbulent eddies decreases. Estimation of particles response functions (25) are made in the sense of following simple expression for the fluid velocity correlation on the particle path

$$\langle E_{ij}(\mathbf{x}, t; \mathbf{R}_p(\xi), \xi) \rangle = \langle u_i u_j \rangle \Delta (T_p - \xi)$$
(42)

where $\Delta(x)$ is the Heaviside step-function.

The calculated particles response functions (25) with assumption (42) have the appearance

$$q_p = 1 - \exp(-T_p/\tau_p), T_p/\tau_p = T_p/(T_{\rm E}\Omega_{\rm E})$$

$$g_p = T_p/\tau_p - \left[1 - \exp\left(-T_p/\tau_p\right)\right]$$
$$p_p = 1 - \left(1 + T_p/\tau_p\right) \exp\left(-T_p/T_p\tau_p\right)$$
$$h_p = 3 + \frac{1}{2} \left(T_p/\tau_p\right)^2 - 2T_p/\tau_p$$
$$- \left(3 + T_p/\tau_p\right) \exp\left(-T_p/\tau_p\right)$$

where $\Omega_{\rm E} = \tau_p / T_{\rm E}$ is the parameter of particles inertia.

5. Boundary conditions for the balance equations of the dispersed phase

5.1. Approximate solution of the PDF equation

For closing the equations system for the first and second moments, Eqs. (31), (32) and (34) are necessary to find expressions for turbulent transfer of momentum and energy of chaotic motion in dispersed phase. Also, we need boundary conditions, representing effect of particles interaction with a wall. For this purpose, we developed the method of an approximate solution of the closed PDF equations (10). This method is similar to the Chapman–Enskog method in the kinetic theory of gases (for example, Cercignani [22]).

In the PDF equations (10) and (28), we consider only the members with first-order of derivatives from particulate phase parameters

$$\frac{\mathbf{D}\langle \Phi \rangle}{\mathbf{D}t} + \left(-\frac{\mathbf{D}\langle V_i \rangle}{\mathbf{D}t} - v_k \frac{\partial \langle V_i \rangle}{\partial x_k} + \frac{\langle U_i \rangle + \tau_p g_i - \langle V_i \rangle}{\tau_p} \right) \frac{\partial \langle \Phi \rangle}{\partial v_i} + v_k \frac{\partial \langle \Phi \rangle}{\partial x_k} - g_p \langle u_i u_k \rangle \frac{\partial^2 \langle \Phi \rangle}{\partial v_i \partial x_k} - \frac{1 - \delta_{ik}}{\tau_p} \sigma_{ik}^0 \frac{\partial^2 \langle \Phi \rangle}{\partial v_i \partial v_k} = \hat{L} \langle \Phi \rangle$$
(43)

$$\frac{\mathbf{D}}{\mathbf{D}t} = \frac{\partial}{\partial t} + \langle V_k \rangle \frac{\partial}{\partial x_k}, \quad \hat{L} = \frac{1}{\tau_p} \frac{\partial}{\partial v_i} v_i + \frac{\sigma_{ii}}{\tau_p} \frac{\partial^2}{\partial v_i \partial v_i}$$
(44)

 $\sigma_{ik}^{\rm o} = q_p \langle u_i u_k \rangle$

where the operator \hat{L} describes the processes of particles chaotic motion generation as a result of particles interaction with turbulent carrying phase velocity and viscous dissipation of random particles motion.

The right-hand side of the Eq. (43) may be inter-

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preted as particles "collision" with turbulent eddies. This collision term is written in the simple Fokker– Plank representation.

We will search the solution of the Eq. (43) in an appearance of expansion with the first correction terms linear on gradients of averaged parameters of the dispersed phase

$$\langle \Phi \rangle = \langle \Phi_0 \rangle + \langle \Phi_1 \rangle$$

The first correction satisfies to normalization restrictions

$$\int \langle \Phi_1 \rangle \, \mathrm{d} \boldsymbol{\nu} = \int v_i \langle \Phi_1 \rangle \, \mathrm{d} \boldsymbol{\nu} = \int v_i v_i \langle \Phi_1 \rangle \, \mathrm{d} \boldsymbol{\nu} = 0$$

The zero-order solution $\langle \Phi_0 \rangle$ of Eq. (43) $\hat{L} \langle \Phi_0 \rangle = \mathbf{0}$, without the account of gradients of averaged parameters, characterize a local-equilibrum situation and have the following form

$$\langle \Phi_0 \rangle = \langle C(\mathbf{x}, t) \rangle \varphi(\mathbf{v}) \tag{45}$$

Here, the PDF of dispersed phase velocity fluctuation $\varphi(\mathbf{v})$ is identical to the expression (38).

For closing the system of equations (31), (32) and (34), we use the zero-order solution (45), and obtain

$$\frac{\mathrm{D}\langle C\rangle}{\mathrm{D}t} + \langle C\rangle \frac{\partial}{\partial x_i} \langle V_i \rangle = 0 \tag{46}$$

$$\frac{\mathrm{D}\langle V_i \rangle}{\mathrm{D}t} + \frac{\partial \sigma_{ii}}{\partial x_i} = \frac{\langle U_i \rangle + \tau_p g_i - \langle V_i \rangle}{\tau_p} - \frac{D_{ii}^{\mathrm{p}}}{\tau_p} \frac{\partial \ln \langle C \rangle}{\partial x_i} \qquad (47)$$

$$\frac{\mathrm{D}\sigma_{ii}}{\mathrm{D}t} + 2\sigma_{ii}\frac{\partial\langle V_i\rangle}{\partial x_i} = \frac{2}{\tau_p} \left(\sigma^{\mathrm{o}}_{ii} - \sigma_{ii}\right)$$
(48)

We suppose that the dispersed phase PDF $\langle \Phi(\mathbf{x}, \mathbf{v}, t) \rangle$ depends on coordinates and time only through averaged parameters

$$\frac{\mathbf{D}\langle \Phi \rangle}{\mathbf{D}t} = \frac{\mathbf{D}\langle C \rangle}{\mathbf{D}t} \frac{\partial \langle \Phi \rangle}{\partial \langle C \rangle} + \frac{\mathbf{D}\sigma_{ii}}{\mathbf{D}t} \frac{\partial \langle \Phi \rangle}{\partial \sigma_{ii}}$$
(49)

With the account of Eqs. (46)–(49), the equation for the first correction $\langle \Phi_1 \rangle$, following from Eq. (43), is given by

$$\Phi_0^{-1} \hat{L} \Phi_1 = \frac{1}{\sigma_{ii}} \left(v_i v_k - \delta_{ik} v_i^2 \right) \frac{\partial \langle V_i \rangle}{\partial x_k} - (1)$$
$$- \delta_{ik} \frac{\sigma_{ik}^0}{\tau_p} \frac{v_i v_k}{\sigma_{ii} \sigma_{kk}} + \frac{v_k}{\sigma_{ii}} \left[\frac{v_i^2}{2\sigma_{ii}} - \left(\delta_{ik} + \frac{1}{2} \right) \right] \frac{\partial \sigma_{ii}}{\partial x_k}$$
(50)

.

By solving Eq. (50), we obtain the PDF approximation with regards to terms containing gradients of the dispersed phase averaged parameters

$$\langle \Phi(\mathbf{x}, \mathbf{v}, t) \rangle = \langle C(\mathbf{x}, t) \rangle \varphi_{\{} 1 + \frac{1}{2} \sigma_{ik}^{o} (1 - \delta_{ik}) \frac{v_{i} v_{k}}{\sigma_{ii} \sigma_{kk}} - \frac{\tau_{p}}{2\sigma_{ii}} (v_{i} v_{k} - \delta_{ik} v^{2}) \frac{\partial \langle V_{i} \rangle}{\partial x_{k}} - \frac{\tau_{p}}{3} v_{k} \bigg[\frac{v_{i}^{2}}{2\sigma_{ii}} - \bigg(\frac{1}{2} + \delta_{ik} \bigg) \bigg] \frac{\partial \ln \sigma_{ii}}{\partial x_{k}} \}$$
(51)

With assistance of the formula (51) we derive expressions representing turbulent transfer of momentum (for $i\neq j$) and intensity of a chaotic motion in the dispersed phase

$$\langle v_i v_j v_k \rangle = -\delta_{ij} \frac{1}{3} (2\delta_{ik} + \delta_{ii}) \tau_p \sigma_{kk} \frac{\partial \sigma_{ii}}{\partial x_k}$$
(53)

5.2. Derivation of boundary conditions

5.2.1. The model of particle-wall collision

With determination of boundary conditions for the balance equations (31), (32) and (34) we rearranged the PDF (51) in a boundary layer approximation $(\partial \langle V_x \rangle / \partial y \gg \partial \langle V_x \rangle / \partial x)$ in the region near the wall

$$\langle \Phi \rangle = \langle C \rangle \varphi \Biggl\{ 1 + \Sigma_{xy} \frac{v_x v_y}{\sigma_{xx} \sigma_{yy}} - \frac{\tau_p}{3} \frac{v_y}{\sigma_{ii}} \Biggl[\frac{v_i^2}{2\sigma_{ii}} - \left(\delta_{iy} + \frac{1}{2} \right) \Biggr] \frac{\partial \sigma_{ii}}{\partial y} \Biggr\}$$

$$(54)$$

$$\Sigma_{xy} = \langle v_x v_y \rangle = q_p \langle u_x u_y \rangle - \frac{\tau_p}{2} \sigma_{yy} \frac{\partial \langle V x \rangle}{\partial y}$$

where the axis y is directed normal to the surface, the

 $\langle \Phi_{\perp}$

axis x coincides with the direction of the stream; Σ_{xy} are turbulent stresses in dispersed phase due to particles turbulence.

We investigated simple model of particle–wall collision. It is supposed that during the particle collision with the wall there is a possible loss of an impulse of the reflected particle. Furthermore, normal velocity of the reflected particle changes its sign

$$V''_{x} = k_{t}V'_{x}, \quad V''_{z} = k_{t}V'_{z}, \quad V''_{y} = -k_{n}V'_{y}$$
(55)

where one prime marks velocity before impact, while two primes, after; k_n, k_t are impulse restitution coefficients.

Moreover, for an impulse loss we involve the probability of particles absorption on the wall, which is described by coefficient χ . If coefficient of particles absorption on the wall is equal to zero $\chi = 0$, all particles touching the wall, do not return in the flow. For $\chi = 1$, particles are not absorbed on the surface.

5.2.2. PDF of reflected particles

From a presumption of equivalence between the fluxes of particles dropping and rebounding from the wall, we can construct the PDF of reflected particles. This PDF is combined by PDF of the dropping particles and shift function, connected with transformation of the incident particles' velocity (44) after the collision

$$V_{y}^{"}\langle \Phi_{+}(\mathbf{x}, \mathbf{V}^{"}, t) \rangle$$

= $-\chi \int_{-\infty}^{\infty} dV_{x}^{\prime} \int_{-\infty}^{0} dV_{y}^{\prime} \int_{-\infty}^{\infty} dV_{z}^{\prime} V_{y}^{\prime} Z_{w}(\mathbf{V}^{"}, \mathbf{V}^{\prime})$
 $\times \langle \Phi(\mathbf{x}, \mathbf{V}^{\prime}, t) \rangle$
 $Z_{w}(\mathbf{V}^{\prime}, \mathbf{V}^{"})$

$$=\delta\left(V_{z}^{"}-k_{t}V_{z}^{"}\right)\delta\left(V_{x}^{"}-k_{t}V_{x}^{\prime}\right)\delta\left(V_{y}^{"}+k_{n}V_{z}^{\prime}\right)$$
(56)

In the case of an absolutely elastic surface $k_n = k_t = 1$ from the expression (56), it follows that

$$\langle \Phi_+(\mathbf{x}, V_x, V_y, V_z, t) \rangle = \chi \langle \Phi(\mathbf{x}, V_x, -V_y, V_z, t) \rangle,$$

$$V_y > 0$$

This boundary condition for PDF agrees well, for example, with a condition accepted by Menon et al. [14] for a comparatively absorbing surface.

Utilizing the formulas (54) and (56) we find closed expression for particles PDF reflected from the wall

$$(\mathbf{x}, \mathbf{v}'', t)$$

$$= \frac{k}{k_n} \langle C \rangle \varphi'' \left\{ 1 - \sum_{xy} \frac{x \cdot y}{k_l k_n \sigma_{xx} \sigma_{yy}} + \frac{\tau_p}{3} \frac{v_y''}{k_n} \left[\left(\frac{v_x''^2}{2k_l^2 \sigma_{xx}} - \frac{1}{2} \right) \frac{\partial \ln \sigma_{xx}}{\partial y} + \left(\frac{v_y''^2}{2k_n^2 \sigma_{yy}} - \frac{3}{2} \right) \frac{\partial \ln \sigma_{yy}}{\partial y} + \left(\frac{v_z''^2}{2k_l^2 \sigma_{zz}} - \frac{1}{2} \right) \frac{\partial \ln \sigma_{zz}}{\partial y} \right] \right] \right\}$$
$$\varphi''(\mathbf{v}) = \prod_{i=1}^3 \frac{1}{\left(2\pi k_i^2 \sigma_{ii}\right)^{1/2}} \exp\left(-\frac{v_i''^2}{2k_i^2 \sigma_{ii}} \right)$$
$$v_x'' = V_x'' - k_l \langle V_x \rangle, v_y'' = V_y'' + k_n \langle V_y \rangle, v_z'' = V_z'' \quad (57)$$

 $v''_{...}v''_{...}$

The concentrations of rebounding and dropping particles are

$$\begin{aligned} \langle C_+ \rangle &= \int_{-\infty}^{\infty} \, \mathrm{d}V_x \int_0^{\infty} \, \mathrm{d}V_y \int_{-\infty}^{\infty} \, \mathrm{d}V_z \langle \Phi_+(\boldsymbol{x}, \boldsymbol{V}, t) \rangle \\ &= \frac{\chi}{k_n} \langle C_- \rangle \end{aligned} \tag{58}$$

$$\langle C_{-} \rangle = \int_{-\infty}^{\infty} \mathrm{d}V_{x} \int_{-\infty}^{0} \mathrm{d}V_{y} \int_{-\infty}^{\infty} \mathrm{d}V_{z} \langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle$$
(59)

Taking into consideration the expression for total concentration of particles $\langle C \rangle = \langle C_{-} \rangle + \langle C_{+} \rangle$, we obtain from the formulas (58) and (59) a relation between dropping and reflected particles concentrations near the wall

$$\langle C_{-} \rangle = \frac{k_n \langle C \rangle}{k_n + \chi}, \qquad \langle C_{+} \rangle = \frac{\chi \langle C \rangle}{k_n + \chi}$$
(60)

From formula (60) we can realize that for absorbing surface $\chi = 0$ concentration of dropping particles coincides with the total particles concentration in the flow $\langle C_{-} \rangle = \langle C \rangle (\langle C_{+} \rangle = 0)$. For the absolute nonelastic surface $k_n = 0$, we obtain accumulation of particles on the wall $\langle C_{+} \rangle = \langle C \rangle (\langle C_{-} \rangle = 0)$.

5.2.3. The boundary condition for the dispersed phase concentration

The two-phase dispersed flow can be conditionally separated into two regions. First "near wall region" is located from the surface over the distance about inertial flight of particles moving with their chaotic velocities $0 < y \le l_p \approx \tau_p \sigma^{1/2}$. Second, "external region" is situated beyond the distance about $y > l_p$ from the surface Fig. 1 It is worth noting that in the Eulerian variables the dispersed phase is considered also as a continuous medium. According to this proposition, the inertial flight of particles may be determined as the Eulerian space scale for correlation of dispersed phase velocity fluctuation.

During the process of derivation of boundary conditions for the balance equations, we accept that fluxes of concentration, momentum and turbulent energy of dispersed phase in external region are equal to a sum of the fluxes of corresponding quantities calculated for dropping and reflected particles in the near-wall region. The scale of averaged dispersed phase parameters variation is larger than particles inertial flight l_p . Under this assumption, it is possible to hope that boundary conditions to be found reflect the real picture of formation of dispersed phase averaged parameters. Similar hypothesis for boundary conditions determination was used by Nagvi et al. [12], Protopopescu and Keyes [13] and Menon et al. [14].

The flux of particles concentration toward the wall in the flow is equal

$$F\{\langle C \rangle\} = \int_{-\infty}^{\infty} dV_x \int_{-\infty}^{\infty} dV_y \int_{-\infty}^{\infty} dV_z V_y \langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle$$
$$= \langle C \rangle \langle V_y \rangle$$
(61)

The flux of concentration of particles dropping on the wall is designed as

$$F_{-}\{\langle C \rangle\} = \int_{-\infty}^{\infty} \mathrm{d}V_{x} \int_{-\infty}^{0} \mathrm{d}V_{y} \int_{-\infty}^{\infty} \mathrm{d}V_{z} V_{y} \langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle$$
$$= \frac{\langle C \rangle}{2} \left[\langle V_{y} \rangle - \left(\frac{2}{\pi} \sigma_{yy}\right)^{1/2} \right]$$
(62)

The flux of concentration of particles rebounded from



Fig. 1. The sketch of two regions in the two-phase flow. Arrows show fluxes of particles colliding and reflected from the wall. Dashed lines represent imaging behaviour of dispersed phase concentration outside the flow.

the wall is equal to

$$F_{+}\{\langle C\rangle\} = \int_{-\infty}^{\infty} \mathrm{d}V_{x} \int_{0}^{\infty} \mathrm{d}V_{y} \int_{-\infty}^{\infty} \mathrm{d}V_{z} V_{y} \langle \Phi_{+}(\mathbf{x}, \mathbf{V}, t) \rangle$$
$$= -\chi F_{-}$$
(63)

From the formulas (61)–(63) and balance of concentration fluxes

$$F\{\langle C \rangle\} = F_{-}\{\langle C \rangle\} + F_{+}\{\langle C \rangle\}$$

follow boundary condition for particles concentration

$$\frac{1-\chi}{1+\chi} \left(\frac{2}{\pi} \sigma_{yy}\right)^{1/2} \langle C \rangle = -\langle V_y \rangle \langle C \rangle \tag{64}$$

On the basis of Eq. (32) for the dispersed phase normal velocity component, it is possible to obtain the approximate expression in the near wall region

$$\langle V_{y} \rangle \langle C \rangle = -JC_{m} \approx \underbrace{\left(\langle U_{y} \rangle + \tau_{p}g_{y} \right)}_{I} \langle C \rangle - \underbrace{\tau_{p} \frac{\partial \sigma_{yy}}{\partial y}}_{II} \langle C \rangle$$
$$- \underbrace{D_{yy}^{p} \frac{\partial \ln \langle C \rangle}{\partial y}}_{III} \langle C \rangle \qquad (65)$$

where J is dispersed phase deposition velocity on the wall; $C_{\rm m}$ is particles mean concentration in a cross-section.

Under consideration of Eq. (65), one can notice that normal component of dispersed phase velocity results from the particles motion under gravitational force and velocity of carrying phase in a cross-section, for example, suction/injection (I), the turbophoretic motion associated with nonhomogeneousity of particles turbulent energy (II), and the dispersed phase diffusion velocity due to gradient of particles concentration (III). From Eqs. (64) and (65) it follows that boundary condition (64) combines concentration and gradient of the dispersed phase concentration on the wall.

In the absence of mass force and turbophoresis, the boundary condition (64) corresponds with results obtained earlier in works of Nagvi et al. [12], Protopopescu and Keyes [13], and Menon et al. [14]

$$\frac{1-\chi}{1+\chi} \left(\frac{2}{\pi} \sigma_{yy}\right)^{1/2} \langle C \rangle = D_{yy}^{\rm p} \frac{\partial \langle C \rangle}{\partial y}$$

5.2.4. The boundary condition for the dispersed phase axial velocity

For designing the boundary condition for dispersed phase averaged axial velocity, we calculate momentum flux of particles in the flow and momentum flux of the particles dropping on the wall

$$F\{\langle C \rangle \langle V_x \rangle\}$$
$$= \int_{-\infty}^{\infty} dV_x \int_{-\infty}^{\infty} dV_y \int_{-\infty}^{\infty} dV_z V_y V_x \langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle$$
$$= \langle C \rangle \langle V_y \rangle \langle V_x \rangle$$

 $F_{-}\left\{\langle C\rangle\langle V_{x}\rangle\right\}$ $=\int_{-\infty}^{\infty}dV_{x}\int_{-\infty}^{0}dV_{y}\int_{-\infty}^{\infty}$

$$= \int_{-\infty}^{\infty} dV_x \int_{-\infty}^{\infty} dV_y \int_{-\infty}^{\infty} dV_z V_y V_x \langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle$$
$$= \frac{\langle C \rangle}{2} \left[\langle V_y \rangle \langle V_x \rangle - \left(\frac{2}{\pi} \sigma_{yy}\right)^{1/2} + \Sigma_{xy} \right]$$
(66)

The flux of momentum of particles reflected from the wall is evaluated with application the formula (57) for PDF

$$F_{+}\{\langle C \rangle \langle V_{x} \rangle\}$$

$$= \int_{-\infty}^{\infty} dV_{x} \int_{0}^{\infty} dV_{y} \int_{-\infty}^{\infty} dV_{z} V_{y} V_{x} \langle \Phi_{+}(\mathbf{x}, \mathbf{V}, t) \rangle$$

$$= -\chi k_{t} F_{-}\{\langle C \rangle \langle V_{x} \rangle\}$$
(67)

From Eqs. (66) and (67) and balance between the momentum fluxes

$$J\{\langle C \rangle \langle V_x \rangle\} = J_{-}\{\langle C \rangle \langle V_x \rangle\} + J_{+}\{\langle C \rangle \langle V_x \rangle\}$$

follows the boundary condition for axial velocity of dispersed phase

$$\left[\frac{1-k_t\chi}{1+k_t\chi}\left(\frac{2}{\pi}\sigma_{yy}\right)^{1/2} + \langle V_y\rangle\right]\langle V_x\rangle = \frac{\tau_p}{2}\sigma_{yy}\frac{\partial \langle V_x\rangle}{\partial y}$$
(68)

5.2.5. The boundary condition for the dispersed phase turbulent energy components

Fluxes of particles velocity fluctuations intensity in normal and axial directions in the flow are alike

$$F\{\langle C \rangle \langle v_{y}^{2} \rangle\}$$

$$= \int_{-\infty}^{\infty} dV_{x} \int_{-\infty}^{\infty} dV_{y} \int_{-\infty}^{\infty} dV_{z} V_{y} v_{y}^{2} \langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle$$

$$= \langle C \rangle \left[\langle V_{y} \rangle \sigma_{yy} - \tau_{p} \sigma_{yy} \frac{\partial \sigma_{yy}}{\partial y} \right]$$
(69)

 $F\{\langle C \rangle \langle v_x^2 \rangle\}$ = $\int_{-\infty}^{\infty} dV_x \int_{-\infty}^{\infty} dV_y \int_{-\infty}^{\infty} dV_z V_y v_x^2 \langle \Phi(\mathbf{x}, \mathbf{V}, t) \rangle$

$$= \langle C \rangle \left[\langle V_y \rangle \sigma_{xx} - \frac{\tau_p}{3} \sigma_{yy} \frac{\partial \sigma_{xx}}{\partial y} \right]$$
(70)

The corresponding fluxes for dropping particles look like

$$F_{-}\left\{\langle C\rangle\langle v_{y}^{2}\rangle\right\}$$

$$=\int_{-\infty}^{\infty} \mathrm{d}V_{x}\int_{-\infty}^{0} \mathrm{d}V_{y}\int_{-\infty}^{\infty} \mathrm{d}V_{z}V_{y}v_{y}^{2}\langle\Phi(\mathbf{x},\mathbf{V},t)\rangle$$

$$=\frac{\langle C\rangle}{2}\left[\langle V_{y}\rangle\sigma_{yy}-2\left(\frac{2}{\pi}\sigma_{yy}\right)^{1/2}\sigma_{yy}-\tau_{p}\sigma_{yy}\frac{\partial\sigma_{yy}}{\partial y}\right] (71)$$

$$F_{-}\left\{\langle C\rangle\langle v_{x}^{2}2\rangle\right\}$$

$$=\int_{-\infty}^{\infty} dV_{x}\int_{-\infty}^{0} dV_{y}\int_{-\infty}^{\infty} dV_{z}V_{y}v_{x}^{2}\langle\Phi(\mathbf{x},\mathbf{V},t)\rangle$$

$$=\frac{\langle C\rangle}{2}\left[\langle V_{y}\rangle\sigma_{xx}-2\left(\frac{2}{\pi}\sigma_{yy}\right)^{1/2}\sigma_{xx}\right.$$

$$\left.-\frac{\tau_{p}}{3}\sigma_{yy}\frac{\partial\sigma_{xx}}{\partial y}\right]$$
(72)

Fluxes of chaotic motion intensity in normal and axial directions for rebounding particles are

$$F_{+}\left\{\langle C\rangle\langle v_{y}^{2}\rangle\right\}$$

$$=\int_{-\infty}^{\infty} \mathrm{d}V_{x}\int_{0}^{\infty} \mathrm{d}V_{y}\int_{-\infty}^{\infty} \mathrm{d}V_{z}V_{y}v_{y}^{2}\langle\Phi_{+}(\mathbf{x},\mathbf{V},t)\rangle$$

$$=-\chi k_{n}^{2}F_{-}\left\{\langle C\rangle\langle v_{y}^{2}\rangle\right\}$$
(73)

$$F_{+}\left\{\langle C\rangle\langle v_{x}^{2}\rangle\right\}$$

$$=\int_{-\infty}^{\infty} \mathrm{d}V_{x}\int_{0}^{\infty} \mathrm{d}V_{y}\int_{-\infty}^{\infty} \mathrm{d}V_{z}V_{y}v_{x}^{2}\langle\Phi_{+}(\mathbf{x}, \mathbf{V}, t)\rangle$$

$$=-\chi k_{t}^{2}F_{-}\left\{\langle C\rangle\langle v_{x}^{2}\rangle\right\}$$
(74)

We applied the formulas (69), (71) and (73), and accordingly (70), (72) and (74) to the following conditions of equality for fluxes

$$F\{\langle C\rangle\langle v_y^2\rangle\} = F_-\{\langle C\rangle\langle v_y^2\rangle\} + F_+\{\langle C\rangle\langle v_y^2\rangle\}$$
$$F\{\langle C\rangle\langle v_x^2\rangle\} = F_-\{\langle C\rangle\langle v_x^2\rangle\} + F_+\{\langle C\rangle\langle v_x^2\rangle\}$$

The boundary conditions for components of turbulent

energy of dispersed phase in normal and axial directions were obtained

$$\left[\frac{1-k_n^2\chi}{1+k_n^2\chi}2\left(\frac{2}{\pi}\sigma_{yy}\right)^{1/2}+\langle V_y\rangle\right]\sigma_{yy}=\tau_p\sigma_{yy}\frac{\partial\sigma_{yy}}{\partial y}$$
(75)

$$\left[\frac{1-\chi k_t^2}{1-\chi k_t^2} \left(\frac{2}{\pi} \sigma_{yy}\right)^{1/2} + \langle V_y \rangle \right] \sigma_{xx} = \frac{\tau_p}{3} \sigma_{yy} \frac{\partial \sigma_{xx}}{\partial y}$$
(76)

In view of formulas (64), (68), (75) and (76) it is obvious that for completely reflecting surface $\chi = 1$, the flux of the dispersed phase on the wall is absent $\langle V_y \rangle = 0$, and dynamic parameters of the particles are regulated by restitution coefficients. On the elastic surface, $k_n = 1$ and $k_t = 1$, transfer of chaotic motion energy $\partial \sigma_{yy}/\partial y = 0$, $\partial \sigma_{xx}/\partial y = 0$ and axial momentum of particles toward the surface $\partial \langle V_x \rangle/\partial y = 0$ are absent.

The maximum mass transfer of particles on the wall is realized for completely absorbing surface $\chi = 0$. The particles deposition velocity is determined by intensity of particles chaotic motion in the near-wall region

$$J = \left(\frac{2}{\pi}\sigma_{yy}\right)^{1/2} \frac{\langle C \rangle}{C_{\rm m}} \text{ for } y = 0$$

We can remark that on the absorbing surface turbophoretic velocity of particles also reaches the maximum value. A gradient of axial velocity of particles on the absorbing surface disappear, which is linked with an absence in the flow particles reflected from the surface.

6. Conclusions

On the basis of averaging over an ensemble of turbulent realizations, the closed equation for PDF of particles coordinates and velocities in a nonhomogeneous turbulent flow was derived.

The system of equations for dispersed phase concentration, momentum and turbulent energy was written. On the approximate solution of PDF equation, we obtained closed expressions for turbulent transfer of momentum and energy of dispersed phase chaotic motion. These expressions completed the closed equations of turbulent hydrodynamics and mass transfer of dispersed phase in nonhomogeneous flow.

Boundary conditions, taking into account character of particles interaction with a surface, was found. The boundary conditions describe loss of particles impulse during collision with the surface and probability of particles absorption on the surface.

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Appendix A

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The fluctuations of the particle velocity and displacement $v_{pj}(t)$ and $r_{pj}(t)$ depend on carrying phase turbulent velocity $u_k(\mathbf{x}_1, \xi)$ only for times $0 < \xi \le t$. This causal restriction corresponds with equivalence

$$\frac{\delta v_{pj}(t)}{\delta u_k(\mathbf{x}_1, \xi)} = 0 \quad \text{and} \ \frac{\delta r_{pj}(t)}{\delta u_k(\mathbf{x}_1, \xi)} = 0 \quad \text{for } \xi < 0,$$
or $\xi > t$
(A1)

Fluid velocity fluctuations on various directions are approximated by independent random processes. On the basis of definition of functional derivations (Klyatskin [18])

$$\frac{\delta u_i(\mathbf{x}'', t'')}{\delta u_j(\mathbf{x}', t')} = \delta_{ij}\delta(\mathbf{x}'' - \mathbf{x}')\delta(t'' - t')$$
(A2)

expressions (19) and (20) can be completed.

Appendix B

We substitute the expression (38) in the formula (39) and integrate over the dispersed velocity fluctuation. As a result we obtain the following formula for the turbulent fluid velocity autocorrelation function along the particle trajectory

$$\Psi_{p}(\xi) = \frac{1}{A^{3}(\xi)} \exp\left\{-\frac{\xi^{2}}{T^{2}}\left[1 + \frac{W^{2}T^{2}}{L^{2}A^{2}(\xi)}\right]\right\}$$

$$A(\xi) = \left(1 + \frac{2\xi^{2}\sigma}{L^{2}}\right)^{1/2}, \sigma_{ii} = \sigma$$
(B1)

From the formula (B1) it is obvious that growth of relative velocity between phases leads to more intensive attenuation of the turbulent fluid velocity correlation along the particle path.

Integral time scale of the autocorrelation function (B1) characterizes the interaction time of the particle with turbulent eddies

$$T_p = \int_0^\infty \Psi_p(\xi) \,\mathrm{d}\xi \tag{B2}$$

While integrating the expression (B2), we take into

account the slow variations of function $A(\xi)$, compare with exponential term in (B1), and substitute instead of function $A(\xi)$ the constant value $A = A(T_p)$. As a result, we get the non-linear algebraic equation for evaluation of the integral time scale T_p

$$\frac{T_p}{T_E} = \frac{1}{A^3} \left[1 + \left(\frac{WT}{LA}\right)^2 \right]^{-1/2},$$

$$A = \left[1 + 2q_p \left(\frac{T_p u}{L}\right)^2 \right]^{1/2}$$
(B3)

The formula (41) is received by using the notation $uT/L = uT_E/L_E = \gamma/\beta$. For inertial particles without averaged velocity difference between phases, time scale T_p is close to Eulerian integral time scale T_E . In the case of very small particles impurity $(\tau_p \rightarrow 0, q_p \rightarrow 1)$ without relative velocity $\mathbf{W} = 0$ between phases, the time scale T_p (fluid velocity correlation along the passive particle trajectory) conforms to integral Lagrangian time scale $T_p = T_L$. With this assumption, utilizing the formula (B3), we can achieve rough estimation for the ratio of Lagrangian–Eulerian time scale in moving coordinate system

$$\beta = \frac{T_{\rm L}}{T_{\rm E}} = \left(1 + \frac{\pi}{2}\gamma^2\right)^{-3/2}, \quad \gamma = \frac{uT_{\rm L}}{L_{\rm E}}$$
(B4)

From (B4) it is obvious that in the coordinate frame Lagrangian time scale is always less than Eulerian time scale.

For homogeneous turbulence from the formulas (29) and (33), we can determine expression for coefficient of dispersed phase diffusion

$$D_{ii}^{\rm p} = T_p \langle u_i^2 \rangle$$

Coefficient of turbulent diffusion of a passive impurity $\tau_p \rightarrow 0$, (W = 0) is equal to

$$D_{ii}^{\rm o} = T_L \langle u_i^2 \rangle$$

The ratio diffusion coefficients of particles to that of passive impurity is equivalent

$$D_{ii}^{\rm p}/D_{ii}^{\rm o}=T_p/T_L$$

Fig. B1 illustrates effect of relative velocity of particles and parameter of particles inertia $\Omega_{\rm E}$ on the ratio of turbulent diffusion coefficients and on the response function q_p . Function q_p describes intensity of particles turbulent motion. Calculation was made for $\gamma = 0.5$. For inertial particles, coefficient of turbulent diffusion is higher than for passive impurity. The points on Fig. 2 show experimental data of Snyder and Lamley [23] and Wells and Stock [24]. We can declare that at $\gamma = 0.5$ the ratio of Lagrangian–Eulerian time scale in the moving coordinate system is $\beta = T_{\rm L}/T_{\rm E} \approx 0.61$.

Appendix C

Here, we estimate the order of magnitudes of terms in the left- and right-hand sides of the PDF equation (43). The terms in the left part of the Eq. (43) correspond with variation of averaged dispersed phase parameters in time and space. We suppose, that characteristic time scale of variation of averaged parameters exceeds well the particles relaxation time and integral time scale of turbulence. It is also presumed that the characteristic length scale of the two-phase stream cross-section is also significantly greater than integral scale of turbulence $L_0 \gg L_E$.

For low inertial particles $\tau_p \ll T_{\rm E}$, scale of particles inertial flight is about $l_p \approx \tau_p \sigma^{1/2} \approx \tau_p u \ll L_{\rm E}$. In these circumstances we may use the equilibrium approximation, within the framework of which intensity of the particles chaotic motion in a given point depends only on turbulent intensity of the fluid phase in this point vicinity. Thus, the terms in the right-hand side of the Eq. (43) in the operator \hat{L} exceed well the terms in the left-hand side $\epsilon = l_p/L_0 \ll 1$. For this reason, the approximate expansion for PDF with zero order solution (45) is correct.



Fig. B1. The relationship between turbulent diffusion coefficients of inertial particles and passive impurity (a), and response function describing particles turbulent energy (b). Points on Fig. 2(a) are experimental results (Snyder and Lamley [23] and Wells and Stock [23]).

For inertial particles $\tau_p \gg T_{\rm E}$, characteristic length scale of dispersed phase velocity fluctuations is of the order $l_p \approx \tau_p (q_p u^2)^{1/2} \approx (\tau_p T_{\rm E})^{1/2} u$ (formula (26) for function q_p is used). Characteristic length scale of spatial variations of the dispersed phase averaged parameters is about $L_p > L_0 + l_p$ (Menon et al. [14]). Therefore, the terms in the left-hand side of Eq. (43) are lesser than terms in the right-hand side by $\epsilon = l_p/L_p < 1$ times. Hence, for inertial particles the approximate solution of the PDF equation in the expansion is also appropriate.

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