Calculation of probability density function of particle velocity in turbulent flow

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Abstract. The random motion of inertial particles in uniform isotropic turbulence is considered. Fluctuations of the gas velocity at the particle trajectory are modelled as a random Gauss process with a finite decay time of the autocorrelation function. A closed equation for the probability density function (PDF) of the random particle velocity is derived. An analytical solution of the equation for the PDF is found. The equation for the PDF is solved by two numerical methods. The first method of solution is based on the finite-difference approximation of the equation for the PDF. The second method is based on the calculation of empirical PDF, which is obtained by averaging over an ensemble of random trajectories of particles. The results of the comparison of analytical numerical solutions are presented.

1. Introduction

Two-phase turbulent flows are widespread in nature and have numerous technical applications. There are two alternative approaches based on the ideas of Lagrange and Euler. In the Lagrange approach the dynamics of the dispersed phase is calculated on the basis of modelling a huge number of random particle trajectories (of the order of $10^4 - 10^8$). In the Euler approach the system of equations for the dynamics of the dispersed phase is written in the continual approximation. Numerical implementation of the Lagrange approach requires significantly less intellectual effort compared to the Euler approach. However, the processor resources necessary for calculating and storing a huge array of random trajectories of particles in Lagrange variables are significantly higher than those required for calculating the averaged parameters of dispersed phase in Euler method [1-3].

The advantages of the Lagrange and Euler approaches depend on the specific type of problems. For example, if the characteristic residence time of a dispersed turbulent flow in an apparatus is comparable to the characteristic time of dynamic inertia of particles, then the motion of the dispersed phase will be determined by the initial conditions at the entrance to the apparatus. In this case, it is preferable to use the Lagrange method. If the residence time of a dispersed turbulent flow is significantly longer than the integral time scale of turbulence and the particle dynamic timescale, then collective effects associated with turbulent diffusion of particles and collisions of particles between themselves as a result of involvement of the carrier phase in turbulence are important. The only method that can adequately describe collective effects in the dispersed phase is based on the Euler approach [4, 5].

We model gas velocity fluctuations along the particle trajectory as a random Gauss process. Using modern methods of applied functional analysis, we derive a closed equation for PDF of random velocity of particles. The main goal of this paper is present two numerical approaches for solution the PDF.
equation. The first approach is based on the approximation the PDF equation by the finite difference method. The second approach is based on simulation random trajectories of particles. Random trajectories are numerical solution of a system of stochastic ordinary differential equations (SODE). The results of these two numerical approaches are compared with analytical solution of PDF equation.

2. Main equations
We consider a homogeneous isotropic two-phase turbulent gas flow with a small volume concentration of particles, when the influence of particles on turbulence and collisions of particles with each other can be neglected. The motion of an inertial particle occurs as a result of the viscous friction force. The equation for the particle velocity $V(t)$ in the Stokes approximation is

$$\frac{dV(t)}{dt} = -\frac{1}{\tau}[u(X(t),t) - V(t)]$$

Here $\tau$ is particle dynamic relaxation time; $u(x,t)$ is gas velocity fluctuations, whose mean value over an ensemble of turbulent realizations is $\langle u(x,t) \rangle = 0$.

The statistical properties of turbulent fluctuations of the gas velocity on the particle trajectory are assumed to be known $\tilde{u}(t) = u(X(t),t)$. In this case, the equation of particle dynamics takes the form

$$\frac{dV(t)}{dt} = \frac{1}{\tau}[\tilde{u}(t) - V(t)] \quad (1)$$

The direct numerical simulation of turbulence indicates that energy-intensive fluctuations of the gas velocity on the particle trajectory are random Gauss process $\langle \tilde{u}(t')\tilde{u}(t') \rangle = \delta_{tt'} \langle u^2 \rangle \psi(|t' - t'|)$. Integral timescale of gas velocity autocorrelation function $\psi(t)$ is $\tau = \int_0^\infty \psi(s) \, ds$.

3. Equation for PDF
We define the indicator function of the random particle velocity $\varphi(V,t) = \delta(V - V(t))$. Here $\delta(x)$ is Dirac delta-function; $V$ is velocity in the phase space; $V(t)$ is actual velocity of the particle. We obtain the equation for the indicator function

$$\frac{\partial}{\partial t} \varphi(V,t) + \frac{\partial}{\partial V} \left[ \frac{\tilde{u}(t) - V}{\tau} \varphi(V,t) \right] = 0$$

This equation is the Liouville equation that describes the dynamics of the particle velocity in the phase space. PDF of particle velocity $\Phi(V,t)$ follows from averaging the indicator function over the ensemble of turbulent realizations $\Phi(V,t) = \langle \varphi(V,t) \rangle$. Unclosed equation for PDF is

$$\frac{\partial}{\partial t} \Phi(V,t) = \frac{\partial}{\partial V} \left[ \frac{1}{\tau} V \Phi(V,t) \right] - \frac{1}{\tau} \langle \tilde{u}(t) \varphi(V,t) \rangle \quad (2)$$

In the correlation between gas velocity fluctuation and the indicator function we use the Furutsu-Novikov formula [6, 7]

$$\langle \tilde{u}(t)\varphi(V,t) \rangle = \int_0^\infty \langle \tilde{u}(t)\tilde{u}(t') \rangle \left\{ \frac{\delta\varphi(V,t)}{\delta \tilde{u}(t')} \right\} dt'$$

Here $\delta\varphi(V,t)/\delta\tilde{u}(t')$ is functional derivative of the indicator function

$$\frac{\delta\varphi(V,t)}{\delta\tilde{u}(t')} = \frac{\delta}{\delta \tilde{u}(t')} \delta(V - V(t)) = -\frac{\partial\varphi(V,t)}{\partial V} \frac{\delta V(t)}{\delta \tilde{u}(t')}$$
For calculation the functional derivative of the actual velocity of particles, we rewrite equation (1) in the integral form

\[ V(t) = \frac{1}{\tau} \int_0^t e^{-\frac{t-s}{\tau}} \hat{u}(s) \, ds \]

As a result of applying the functional differentiation we calculate correlation involved in the PDF equation (2)

\[ \langle \hat{u}(t) \varphi(V,t) \rangle = -\langle u^2 \rangle \int_0^t e^{-\frac{t-t'}{\tau}} \Psi(t-t') \, dt' \frac{\partial}{\partial V} \Phi(V,t) \]

We introduce the particle velocity response function as

\[ f(t) = \frac{1}{\tau} \int_0^t e^{-\frac{s}{\tau}} \Psi(s) \, ds \] (3)

As a result, we obtain a closed equation for the PDF of a random velocity of particle in a turbulent flow

\[ \frac{\partial \Phi(V,t)}{\partial t} = \frac{\partial}{\partial V} \left\{ \frac{1}{\tau} V \Phi(V,t) \right\} + \frac{\langle u^2 \rangle}{\tau} f(t) \frac{\partial^2 \Phi(V,t)}{\partial V \partial V} \] (4)

Initial distribution of the PDF equation (4) is

\[ \Phi(V,t)\big|_{t=0} = \Phi_0(V) \] (5)

The boundary condition for equation (4) follows from the relation \( \Phi(V,t)\big|_{t \to \infty} \to 0 \). The autocorrelation function of gas velocity oscillations along the particle path is determined by an exponentially decreasing function \( \Psi(t) = \exp(-t/T) \) [8]. In this case, the response function see equation (3) is

\[ f(t) = \frac{1}{\tau} \int_0^t e^{\frac{-s-t}{\tau}} \, ds = \frac{1}{1+\tau/T} \left\{ 1 - \exp\left[ -\frac{t}{\tau} \left( 1 + \frac{\tau}{T} \right) \right] \right\} \]

For sufficiently long times \( t \to \infty \) the response function takes equilibrium value \( f_0 = 1/(1+\tau/T) \).

4. Analytical solution of the equation for PDF

First, we calculate the Green function \( G(V,t|V_0) \) for the equation (4). Equation for Green function is

\[ \frac{\partial}{\partial t} G(V,t|V_0) = \frac{\partial}{\partial V} \left\{ \frac{1}{\tau} V G(V,t|V_0) \right\} + \frac{\langle u^2 \rangle}{\tau} f(t) \frac{\partial^2}{\partial V^2} G(V,t|V_0) \quad G(V,t|V_0)\big|_{t=0} = \delta(V-V_0) \]

We find the expression for the Green function

\[ G(V,t|V_0) = \frac{1}{\sqrt{2\pi \langle v^2(t) \rangle}} \exp\left\{ -\frac{\left[ V - V_0 \exp(-t/\tau) \right]^2}{2 \langle v^2(t) \rangle} \right\} \]

Here Green function \( G(V,t|V_0) \) represents the particle velocity \( V \) at time \( t \), if at the initial time \( t = 0 \) the particle velocity is \( V_0 \); \( \langle v^2(t) \rangle \) is dispersion of particle random velocity

\[ \langle v^2(t) \rangle = f_0 \langle u^2 \rangle \left\{ \frac{1+\tau/T}{1-\tau/T} \exp\left( -\frac{2t}{T} \right) + 1 - \frac{2}{1-\tau/T} \exp\left[ -\frac{t}{T} \left( 1 + \frac{\tau}{T} \right) \right] \right\} \] (6)

For an arbitrary initial velocity distribution, see equation (5), the solution of the equation (4) for the PDF is written through the Green function.
\[ \Phi(V,t) = \int G(V,t|V') \Phi_0(V') \, dV' \]

The initial distribution of the particle velocity we set as Gaussian function

\[ \Phi_0(V) = \frac{1}{\sqrt{2\pi \sigma_0^2}} \exp \left\{ -\frac{(V-V_0)^2}{2\sigma_0^2} \right\} \]

The PDF of the particle velocity distribution has the form

\[ \Phi(V,t|V_0) = \frac{1}{\sqrt{2\pi (w^2(t))}} \exp \left\{ -\frac{[V-V_0 \exp(-t/\tau)]^2}{2\langle w^2(t) \rangle} \right\}, \quad \langle w^2(t) \rangle = \langle v^2(t) \rangle + \sigma_0^2 \exp(-2t/\tau) \quad (7) \]

5. Finite difference numerical integration

Consider the general form of the PDF equation

\[ \frac{\partial \Phi(X,t)}{\partial t} + \frac{W(X,t)}{\partial X} = 0, \quad W(X,t) = F(X) \Phi(X,t) - G(X) \frac{\partial}{\partial X} \left[ f(X,t) G(X) \Phi(X,t) \right] \quad (8) \]

Here \( W(X,t) \) is a probability flux.

In the numerical implementation the variable range is limited \( X_{\text{min}} \leq X \leq X_{\text{max}} \). The PDF satisfies the normalization condition

\[ \int_{X_{\text{min}}}^{X_{\text{max}}} \Phi(X,t) \, dX = 1, \quad \int_{X_{\text{min}}}^{X_{\text{max}}} \Phi_0(X) \, dX = 1 \]

To preserve the normalization condition, we require that the probability flows vanish at the boundaries of the region \( W(X,t)|_{X_{\text{min}}} = W(X,t)|_{X_{\text{max}}} = 0 \).

To construct a conservative difference scheme, we integrate equation (8) over the unit cell \([X_{i-1/2}, X_{i+1/2}] \times [t_n, t_n + \Delta t] \), and write down the numerical scheme

\[ \frac{\Phi^{(i+1)} - \Phi^{(i)}}{\Delta t} + \left( \frac{F_{i+1/2}^{(i)}}{\Phi^{(i+1)/2}} - \frac{F_{i-1/2}^{(i)}}{\Phi^{(i-1)/2}} \right) = \frac{1}{h_i} \left[ G_{i+1/2}^{(i)} \left( \frac{f_{i+1} G_{i+1} \Phi_{i+1} - f_{i} G_{i-1} \Phi_{i-1}}{h_{i+1/2}} \right) - G_{i-1/2} \left( \frac{f_{i} G_{i} \Phi_{i-1} - f_{i+1} G_{i+1} \Phi_{i+1}}{h_{i-1/2}} \right) \right] \quad (9) \]

The convective term is modeled to preserve the diagonal dominance

\[ \Phi_{i+1/2} = \theta_{i+1/2} \Phi_i + (1 - \theta_{i+1/2}) \Phi_{i-1}, \quad \theta_{i+1/2} = \left( 1 + \left| \frac{F_{i+1/2}}{F_{i-1/2}} \right| \right) / 2 \]

With this method depending on the sign \( F_{i+1/2} \) we automatically obtain an approximation along the flow, or against the flow. For approximation boundary conditions at the points \( i = 0, i = N \), we integrate equation (8) over “half-integer” cells \([X_{i-1/2}, X_{i+1/2}] \times [t_n, t_n + \Delta t] \), \([X_{N-i-1/2}, X_{N-i+1/2}] \times [t_n, t_n + \Delta t] \). As a result, we write down approximation for the boundary conditions as

\[ \frac{\Phi_0^{(i+1)} - \Phi_0^{(i)}}{\Delta t} + \frac{2}{h_{1/2}} \left( \frac{F_{1/2}^{(i+1/2)}}{\Phi_{1/2}^{(i+1/2)}} - G_{1/2}^{(i)} \left( \frac{f_{1} G_{1} \Phi_{1} - f_{0} G_{0} \Phi_{0}}{h_{1/2}} \right) \right) = 0 \quad (10) \]

\[ \frac{\Phi_{N-i}^{(i+1)} - \Phi_{N-i}^{(i)}}{\Delta t} - \frac{2}{h_{N-i/2}} \left( \frac{F_{N-i/2}^{(N-i-1/2)}}{\Phi_{N-i/2}^{(N-i-1/2)}} - G_{N-i/2}^{(N-i)} \left( \frac{f_{N-i} G_{N-i} \Phi_{N-i} - f_{N-i-1} G_{N-i-1} \Phi_{N-i-1}}{h_{N-i/2}} \right) \right) = 0 \quad (11) \]
Equation (9), (10) and (11) approximate the PDF equation (8) with accuracy \( O(\Delta t + h^2) \).

6. Numerical integration of SODE

Empirical PDF is obtained by averaging an ensemble of random trajectories of particles. The system of differential equations describing the color noise of gas and particle velocity fluctuations are

\[ \frac{d\tilde{u}(t)}{dt} = \frac{1}{\tau} [\eta(t) - \tilde{u}(t)] \]  
\[ \frac{dV(t)}{dt} = \frac{1}{\tau^2} [\tilde{u}(t) - V(t)] \]

Here \( \eta(t) \) is Gauss white noise that generates the computer

\[ \eta(t) = \tau \eta(t - \Delta t) \]

We use a modern method of integrating a system of stochastic differential equations based on the Runge–Kutta algorithm. Stochastic differential equation in the Ito form is

\[ d\mathbf{X}(t) = \mathbf{A}(\mathbf{X}(t), t) dt + \mathbf{B}(\mathbf{X}(t), t) d\mathbf{W}(t) \]

Here \( d\mathbf{W}(t) \) is increment of the Wiener process.

The Runge–Kutta method upgraded for SODE consists of predictor and corrector steps [9,10]

\[ \mathbf{x}_i = \mathbf{x}_i^{(n)} + \Delta t \sum_{j=1}^{N} \hat{R}_j \mathbf{A}(\mathbf{x}_j, t_n) + \Xi \sum_{j=1}^{N} \hat{R}_j \mathbf{B}(\mathbf{x}_j, t_n), \quad \mathbf{x}_i^{(n+1)} = \mathbf{x}_i^{(n)} + \Delta t \sum_{j=1}^{N} r_j \mathbf{A}(\mathbf{x}_j, t_n) + \Xi \sum_{j=1}^{N} r_j \mathbf{B}(\mathbf{x}_j, t_n) \]

Here \( \Xi = \sqrt{\Delta \xi} \); \( \xi \) is a random variable having a Gaussian distribution with a zero mean value and a unit variance; matrices \( \hat{R}_j \) and \( R_j \) are given by the Butcher table.

The solution of the SODE equation (12) and (13) represents the actual values of the velocities of gas and particles and can be considered as a numerical experiment. With a sufficiently large number of particles in the ensemble we calculate empirical PDF.

7. Calculation results

Here we present the results of calculations of the intensity of particle velocity fluctuations and the autocorrelation function for particles and gas.

![Figure 1](image-url)

**Figure 1.** Comparison of direct numerical simulation results (points) with analytical formulas [11] (lines): \( 1 - \tau = 0; 2 - \tau/T = 1; 3 - \tau/T = 3; 4 - \tau/T = 5 \).

We determine the equilibrium autocorrelation function of particle velocity fluctuations \( \Psi_p(t) \) as

\[ \langle V(t') V(t') \rangle = \langle v^2 \rangle \Psi_p(t' - t') \]

(\( \langle v^2 \rangle \) is equilibrium dispersion of particles velocity fluctuations).
In [11] for equation (12) and (13) expressions for the dispersion of velocity fluctuations and the autocorrelation function of particles were obtained. From figure 1 it can be seen that the results obtained by various methods are in satisfactory agreement ($\Psi$ is autocorrelation function of particle velocity fluctuations). We present a comparison of two numerical methods for solving one dimensional variant of the equation (4) with an analytical solution, see equation (6) and (7). Figure 2 illustrates the comparison of the analytical solution with the result of integrating the PDF equation (8) by the finite difference method and by direct numerical simulation.

![Figure 2. Comparison of PDFs obtained on the basis of an analytical solution (line), using the finite difference method (point) and direct numerical simulation (histogram) for different moments of time: $t/T = 1 - 0; 2 - 1; 3 - 3; 4 - 5; 5 - 23$. The dimensionless dynamic relaxation time of particles is $\tau/T = 1, 3, 5$.](image)

**Conclusions**
The paper presents two numerical methods for solving a closed nonstationary equation for the PDF of the random velocity of particles. Calculation methods are based on principally different approaches. In the first case, the traditional method of numerical integration of the equation for PDFs based on the finite difference method is used. The second approach uses a numerical experiment based on the integration of the SODE system.

A technique is proposed that allows one to simulate random fluctuations of the gas velocity as a Gauss process with a given autocorrelation function. A comparison was made between analytical results and direct numerical simulation for autocorrelation function and velocity dispersion of particles.

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**References**
[1] Minier J P, Próżeta C 2015 *Phys. Rev. E - Stat. Nonlinear, Soft Matter Phys* **92** 1
[2] Reeks M, Swailes D, Bragg A 2018 *Phys. Rev. E*. **97** 1
[3] Chibbaro S, Minier J 2008 *J. Aerosol Sci.* **39** 555
[4] Derevich I 2000 *Int. J. Heat Mass Transf.* **43** 3709
[5] Risken H 1989 *The Fokker-Planck equation* (Berlin, Hedelberg: Springer-Verlag)
[6] Hasegawa H 2008 *Phys. A Stat. Mech. its Appl.* **387** 2697
[7] Liang G, Cao L and Wu D 2004 *Phys. A Stat. Mech. its Appl.* **335** 371
[8] Wetchagaruna S, Riley J 2010 *Phys. Fluids*. **22** 063301-1
[9] Burrage K, Burrage P 1996 *Appl. Numer. Math.* **22** 81
[10] Debrabant K, Rößler A 2008 *Math. Comput. Simul.* **77** 408
[11] Derevich I 2015 *Thermophys. Aeromechanics*. **22** 151