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To the Problem of Turbulent Diffusion Instability

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The paper proposes the statistical model of diffusion instability between particles making Brownian motion in incompressible medium. The expression of the perturbed concentration of impurities has been derived on the basis of the stochastic integro-differential equation containing potential energy between interacting particles using the Picard method. Effective diffusion coefficient is derived containing both molecular and turbulent diffusion coefficients. The condition of the negative diffusion instability has been revealed at which impurity cells can be attracted and repelled depending on the potential energy sign. Effective potential energy between the interacting spherical liquid elements has been obtained, which can lead to the instability. The effect of the "Turbulent Diffusion Instability" has been revealed for the first time. The obtained results are valid for an arbitrary autocorrelation tensor of the velocity pulsations.

Keywords: Diffusion instability, stochastic integro-differential equation, turbulence, statistical moments.

AMS Subject Classification: 76F55, 60H15, 60J60.

1. Introduction

Waves propagation in random media has been well investigated [1, 2]. Peculiarities of the statistical characteristics of scattered electromagnetic waves in the terrestrial atmosphere and ionosphere have been considered in [3–7]. The features of turbulent diffusion based on a stochastic equation with random coefficients are investigated in this paper. This approach is universal, allowing to investigate problems of various types, different characteristics of the environment and boundary conditions.

The most important and most commonly used theory of turbulent diffusion is the theory based on the parabolic-type diffusion equation in partial derivatives for the average concentration of diffusive impurity. Different theoretical ideas of the turbulent diffusion processes were proposed in [8, 9]. Mass transfer processes in the atmosphere are realized by molecular and convective turbulent diffusion in liquid and gases. It was established experimentally that integer groups of molecules are characterized by mixing lengths and turbulent viscosity participate in mixing processes of turbulent flows, contrary to the laminar streams. Turbulence favors the mixing of different impurities in different media. Interaction of impurities leads to

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the temporal evolution of medium inhomogeneous structure. Medium passes to the metastable state with various developing relaxation processes. Inhomogeneities can lead both to the velocity pulsation and changing of diffusing processes direction, to the appearance of local instabilities retaining the other region of the system in equilibrium state. Under the term "impurities" further we shall imply both particles and the clusters of molecules.

Stochastic differential equations can be used to describe turbulent diffusion, and this approach makes it easy to construct a number of generalized and modified classical theories based on parabolic-type diffusion equations. A new statistical model of the turbulent diffusion is proposed in this paper, where potential energy between diffusing impurities plays a key role.

2. Distribution of the passive impurities in a turbulent flow

Let us consider mean concentration distribution of the passive impurities using the effective medium approximation. Concentration $N(\mathbf{r},t)$ and velocity $\mathbf{V}(\mathbf{r},t)$ of incompressible medium satisfy the equation

$$\frac{\partial N}{\partial t}+\frac{\partial}{\partial x_\alpha}(NV_\alpha)-D\ \Delta N=S(\mathbf{r},t). \tag{1}$$

Source of impurity $S(\mathbf{r},t)$ is an arbitrary deterministic function of coordinate and time, D is the coefficient of the molecular diffusion. Submit functions N and $\mathbf{V}$ as a sum of slowly varying functions and fluctuating terms, which are random functions of coordinates and time

$$N(\mathbf{r},t)=N_0(\mathbf{r},t)+n(\mathbf{r},t),\ \ \mathbf{V}(\mathbf{r},t)=\mathbf{V}_0+\mathbf{u}(\mathbf{r},t),\ \ V_0=\text{const}.$$

The set of equations for the mean and fluctuating concentrations ($N_0\gg n$) can be written as

$$\frac{\partial N_0}{\partial t}+V_{0\alpha}\frac{\partial N_0}{\partial x_\alpha}-D\frac{\partial^2 N_0}{\partial x_\alpha^2}=-\frac{\partial}{\partial x_\alpha}<nu_\alpha>+S(\mathbf{r},t),$$

$$\frac{\partial n}{\partial t}+V_{0\alpha}\frac{\partial n}{\partial x_\alpha}-D\frac{\partial^2 n}{\partial x_\alpha^2}=-\frac{\partial}{\partial x_\alpha}<u_\alpha N_0>.$$

Here $\alpha=x,y,z$. Taking into account the initial condition $n(\mathbf{k},0)=0$ we have

$$n(\mathbf{k},t)=ik_\beta\exp[-a(k)t]\int\limits_0^t dt'\exp[a(k)t']\int\limits_{-\infty}^{\infty}d\mathbf{k}'u_\beta(\mathbf{k}-\mathbf{k}',t')N_0(\mathbf{k}',t'),$$

where $a(k)=ik_\alpha V_{0\alpha}+Dk^2$.

$3D$ spectral density of the mean concentration of the passive impurity satisfies the intego-differential equation

$$\frac{\partial N_0(\mathbf{k},t)}{\partial t}+b(k)N_0(\mathbf{k},t)=S(\mathbf{k},t), \tag{2}$$

where $b(k) = ik_\alpha V_{0\alpha} + k^2 D_{\text{eff}}(\mathbf{k})$; effective diffusion coefficient for an arbitrary autocorrelation tensor of the velocity pulsations $W_{\alpha\beta}(\boldsymbol{\rho}, \tau)$ can be written as

$$D_{\text{eff}}(\mathbf{k}) = D + \frac{< u^2 >}{(2\pi)^3} \frac{k_\alpha k_\beta}{k^2} \int\limits_{-\infty}^{\infty} d\mathbf{k}' \int\limits_{-\infty}^{\infty} d\boldsymbol{\rho} \int\limits_{0}^{\infty} d\tau W_{\alpha\beta}(\boldsymbol{\rho}, \tau) \exp[-i(\mathbf{k} - \mathbf{k}')\boldsymbol{\rho} - a(k')\tau].$$

For solenoidal velocity ($k_\alpha W_{\alpha\beta}(\mathbf{k}, t) = k_\beta W_{\alpha\beta}(\mathbf{k}, t) = 0$) using the initial conditions, the solution of equation (2) may be written as

$$N_0(\mathbf{r}, t) = \int\limits_{-\infty}^{\infty} d\mathbf{k} \exp[i\mathbf{k}\mathbf{r} - b(k)t] \int\limits_{0}^{t} dt' S(\mathbf{k}, t') \exp[b(k)t'].$$

3. Effective diffusion coefficient

The evolution of the impurity concentration caused by both molecular and turbulent diffusions is carried out on the basis of equation (1) applying the continuity equation of an incompressible liquid. Using the average field method [1, 2], the set of equations for the mean and fluctuating terms of impurity concentration in the first order approximation has the following form

$$Q(\mathbf{k}, \omega) N_0(\mathbf{k}, \omega) = ik_\alpha \int d\mathbf{k}' \int\limits_{-\infty}^{\infty} d\omega' < n(\mathbf{k}', \omega') u_\alpha(\mathbf{k} - \mathbf{k}', \omega - \omega') >= S(\mathbf{k}, \omega),$$

$$Q(\mathbf{k}, \omega) n(\mathbf{k}, \omega) = -ik_\beta \int d\mathbf{k}' \int\limits_{-\infty}^{\infty} d\omega' N_0(\mathbf{k}', \omega') u_\beta(\mathbf{k} - \mathbf{k}', \omega - \omega'), \qquad (3)$$

$$k_\alpha u_\alpha(\mathbf{k}, \omega) = 0,$$

where $Q(\mathbf{k}, \omega) = -i(\omega - \mathbf{k}\mathbf{V}_0) + k^2 D + \frac{\mu}{U_0} k^2 \Pi(\mathbf{k})$.

The solution of the set of equations (3) yields the effective diffusion coefficient

$$D_{\text{eff}}(\mathbf{k}, \omega) = D + \frac{\mu}{M_0} \Pi(\mathbf{k}) + \frac{k_\alpha k_\beta}{k^2} \int d\mathbf{k}' W_{\alpha\beta}(\boldsymbol{\kappa}, \Omega) \equiv D_{\text{eff}}^{\text{mol}}(k) + D_{\text{eff}}^{\text{turb}}(\mathbf{k}, \omega), \quad (4)$$

where $\boldsymbol{\kappa} = \mathbf{k} - \mathbf{k}'$, $\Omega = \omega - (\mathbf{k}'\mathbf{V}_0) + i\mathbf{k}'^2 D_{\text{eff}}^{\text{mol}}(\mathbf{k}')$.

It contains both molecular and turbulent diffusion coefficients and the potential energy of interacting impurities. Effective turbulent diffusion coefficient depends on a characteristic spatial (l) and temporal (T) scales of medium velocity pulsations, as well as on the direction of a turbulent flow. This means that a turbulent diffusion coefficient is anisotropic. Formula (4) is valid for an arbitrary spatial-temporal second rank correlation tensor $W_{\alpha\beta}(\boldsymbol{\kappa}, \Omega)$ of a turbulent velocity field.

4. Diffusion instability of interacting particles

Turbulence has been caused by concentration gradient of molecules clusters, convection transfer of inhomogeneities and potential field gradient induced by other impurities of inhomogeneous medium in a given space point. Conservation condition of matter, taking the interaction of diffusible particles into account, may be written as:

$$\frac{\partial N(\mathbf{r},t)}{\partial t}+\frac{\partial}{\partial x_\alpha}(NV_\alpha)-D\frac{\partial^2 N}{\partial x_\alpha^2}$$
$$=\frac{\mu}{U_0}\nabla\left\{1+\sum_{n=1}^{\infty}\frac{1}{n!}\lambda^n[N^{(n-1)}-1]\nabla\right\}\int\limits_{-\infty}^{\infty}d\mathbf{r}'\Pi(\mathbf{r}-\mathbf{r}')N(\mathbf{r}',t)+S(\mathbf{r},t),$$

where D and μ are molecular diffusion and mobility, respectively; $\mathbf{V}$ is a medium velocity; U_0 is a volume of a unit cell; $\Pi(\mathbf{r}-\mathbf{r}')$ is the potential energy between two interacting impurities located in $\mathbf{r}$ and $\mathbf{r}'$ points. In the absence of interaction uniform distribution of the particle is stable

$$\lim_{t\to\infty}N(\mathbf{r},t)=\text{const}\quad\text{and}\quad\lim_{U_0\to\infty}\frac{1}{U_0}\int\limits_{U_0}d\mathbf{r}N(\mathbf{r},t)=\text{const}<\infty;$$

$\alpha=x,y,z$; $S(\mathbf{r},t)$ is a deterministic function of impurity distribution appearing or disappearing per unit of volume and per unit of time; λ is an arbitrary constant parameter and in final results it will be set to one. Using the Picard iteration method [10] we will seek the solution of equation (1) in a series as a sum of the mean and fluctuating terms: $N(\mathbf{r},t)=N_0(\mathbf{r},t)+\lambda n(\mathbf{r},t)+\lambda^2N^{(2)}(\mathbf{r},t)+\cdots$, $N_0\gg n$, $\mathbf{V}(\mathbf{r},t)=\mathbf{V}_0+\mathbf{u}(\mathbf{r},t)$, $V_0=\text{const}$. The second terms are random functions of the spatial coordinates and time with zero average mean values. Taking into account the incompressibility equation $\partial u_\alpha/\partial x_\alpha$, we obtain

$$\left[-i(\omega-\mathbf{kV}_0)+Dk^2\right]n(\mathbf{k},\omega)+\frac{\mu}{U_0}\int\limits_{-\infty}^{\infty}d\mathbf{k}'\int\limits_{-\infty}^{\infty}d\omega'\{[k^2-(\mathbf{kk}')]\Pi(\mathbf{k}-\mathbf{k}')$$
$$+(\mathbf{kk}')\Pi(\mathbf{k})\}N_0(\mathbf{k}',\omega')n(\mathbf{k}-\mathbf{k}',\omega-\omega')$$
$$=-ik_\alpha\int d\mathbf{k}'\int\limits_{-\infty}^{\infty}d\omega'N_0(\mathbf{k}',\omega')u_\alpha(\mathbf{k}-\mathbf{k}',\omega-\omega'). \quad (5)$$

For a solenoidal incompressible, stationary velocity field ($(k_\alpha u_\alpha)=0$) and $N_0=$ const equation (5) reduces to the dispersion equation

$$\omega=(\mathbf{kV}_0)-ik^2\left[D+\frac{\mu N_0}{U_0}\Pi(\mathbf{k})\right].$$

In this case perturbation of an impurity concentration at arbitrary moment can be written as

$$n(\mathbf{r},t) = \int\limits_{-\infty}^{\infty} d\mathbf{k}\; n(\mathbf{k}) \exp\left\{ i\mathbf{kr} - i(\mathbf{kV}_0)t - ik^2 \left[D + \frac{\mu N_0}{U_0}\Pi(\mathbf{k}) \right] \right\}.$$

If $\min\limits_k \Pi(\mathbf{k}) > 0$ it is possible to introduce the effective diffusion coefficient $D_* = D + \mu N_0 \Pi(\mathbf{k})/U_0$, but at $\min\limits_k \Pi(\mathbf{k}) < 0$ there exists a limiting value of impurity concentration:

$$N_{0*} = -\frac{DU_0}{\mu \min\limits_k \Pi(\mathbf{k})}$$

starting from which ($N_0 > N_{0*}$) negative diffusion instability arises. Generally, U_0 and $\Pi(\mathbf{k})$ are functions of the temperature T_0 and, therefore, N_{0*} is a nonlinear function of T_0. Without loss of generality, lets consider two clusters of molecular impurity with increasing (n_1) and decreasing (n_2) concentration perturbation, $n_1 > n_2$. Coordinate x_0 corresponds to the inflection point of the function $n(x)$, i.e., $(\partial^2 n/\partial x^2)\big|_{x=0} = 0$. This is a boundary between two cells, along which concentration perturbation does not change. Critical value of non-excited impurity

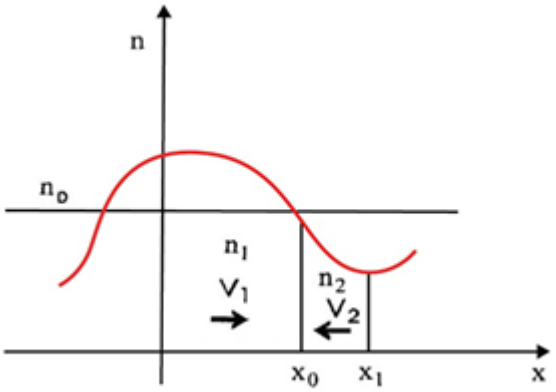

Figure 1. Pattern of diffusion instability

concentration N_0 is determined by the instability criterion. At $N_0 > N_{0*}$ the first cell additionally densifying at the expense of depletion of a second one. In the region where inequality $0 < x < x_0$ is fulfilled, the function $n(x)$ is convex upward $(\partial^2 n/\partial x^2) = 0$. Impurity concentration must be increased $(\partial n_1/\partial t) > 0$. Hence, the diffusion instability appears in the first cell at $D_* < 0$. In the region where the condition $x_0 < x < x_1$ is satisfied, the function $n(x)$ is convex downwards $(\partial^2 n/\partial x^2) > 0$. According to the condition of instability the inequality $(\partial n_2/\partial t) < 0$ must be satisfied. Diffusion instability in the second cell will take place at $D_* < 0$. Effective diffusion coefficient is negative for both cells. Consequently, the analytical form of the potential energy of interacting impurity particles or clusters of different kind of molecules plays an important role in diffusion

instability evaluation. In the region where the inequality $0 < x < x_0$ is fulfilled, the function $n(x)$ is convex upward $(\partial^2 n/\partial x^2) = 0$. Impurity concentration must increase $(\partial n_1/\partial t) > 0$. Hence, the diffusion instability appears in the first cell at $D_* < 0$. In the region where the condition $x_0 < x < x_1$ is satisfied, the function $n(x)$ is convex downwards $(\partial^2 n/\partial x^2) > 0$. According to the condition of instability, the inequality $(\partial n_2/\partial t) < 0$ must be satisfied. Diffusion instability in the second cell will take place at $D_* < 0$. Effective diffusion coefficient is negative for both cells. If impurities during the period of diffusion instability are involved in any chemical reactions, then it is impossible to introduce the concept of an effective diffusion coefficient associated with their interaction with each other. Therefore, the analytical type of potential energy of interaction between impurity particles or liquid elements plays an important role in the development of diffusion instability. Consequently, the analytical form of the potential energy of interacting impurity particles or clusters of different kind of molecules plays an important role in diffusion instability evaluation. This is the diffusion instability effect.

Long range interaction between Brownian particles was considered in [11]. We define the effective interaction potential $\Pi(k)$ between the Brownian particles. A weak, slowly decreasing interaction with the distance occurs between particles making a Brownian movement in a viscous liquid. When the particle moves, it causes movement in the surrounding layers of liquid, which in turn can affect neighboring particles and also set them in motion. The relative displacement of particles in the environment of the remaining particles is characterized, along with a chaotic, defined regular part. The joint movement of particles occurs as if there were quite deterministic forces between them, depending in general on the distance and on the shape of the particles. Calculations show that at small Reynolds numbers, spherical particles with radii R_1 and R_2 repel one another with an average force $\mathbf{F} = -\nabla\Pi$. Effective potential of interacting particles is

$$\Pi(r) = \frac{9}{16}\frac{R_1 R_2}{|\mathbf{r_1} - \mathbf{r_2}|^2} k_B T_0 \tag{6}$$

decreasing with distance as r^{-2} and the energy of this interaction is less than $k_B T_0$; k_B is the Boltzmanns constant, $\mathbf{r_1}$ and $\mathbf{r_2}$ are radius vectors determining the position of the centers of the first and second particles, respectively. At big distances between particles, the repulsive force is inversely proportional to the cube of the distance. The Fourier transformation of (6) $\Pi(k) = 9\pi^2 R_1 R_2 k_B T_0/8k$ is always positive and, therefore, diffusion instability does not occur in this case.

Using similarity method, we suggest the new potential energy between the diffusion particles

$$\Pi(r) = \frac{U_1 U_2}{|\mathbf{r_1} - \mathbf{r_2}|^3} k_B T_0.$$

Fourier transformation can be written as

$$\Pi(k) = 4\pi (U_1 U_2)^{1/2} k_B T_0 [\cos(kR) Si(kR) - \sin(kR) Ci(kR)] \frac{1}{kR},$$

where R is a minimal distance between the interacting clusters having volumes U_1 and U_2; $Si(x)$ and $Ci(x)$ are integral sine and cosine. At small kR the curve has

a shape of the potential hole, i.e., spherical liquid elements are attracted to each other. Increasing the parameter kR, function $\Pi(k)$ oscillates near the zero level.

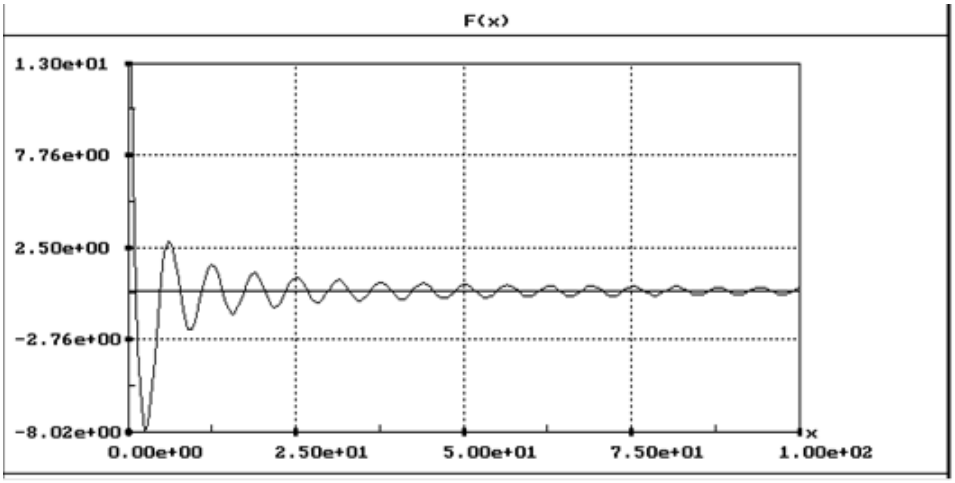

Figure 2. The dependence of the potential energy versus parameter kR

This means that liquid elements are periodically attracted and repelled. Using the asymptotic expressions of the functions $Si(x)$ and $Ci(x)$ we obtain

$$\Pi(k) \sim -4\pi(U_1U_2)^{1/2}\frac{k_BT_0}{(kR)^2}.$$

Effective potential energy of two interacting cells is negative which may cause negative diffusion instability.

5. Conclusion

Based on the stochastic impurity transfer equation or molecular clusters with variable coefficients, the effect of their interaction on the nature of diffusion change is studied. The concentration of impurities and the velocity of their movement is a random function of spatial coordinates and time. The Picard method obtained a set of stochastic differential equations for incompressible fluid that take into account the potential energy of interacting elements. The turbulent diffusion coefficient is calculated containing both molecular and turbulent diffusion coefficients. These expressions are valid for the arbitrary correlation function of the velocity fluctuation of molecular clusters with spatial-temporal scales of turbulence considering the potential energy of their interaction. A condition was found under which impurity particles are attracted to each other, which causes a new effect of the "Diffusion Instability." In this case, the potential energy has the form of a potential hole, and then oscillates to both positive and negative values, which correspond to the repulsion and attraction of diffuse impurities.

The description of the turbulent diffusion in terms of the stochastic differential equations is very convenient for numerical modeling; such modeling can also be considered as a general method of numerical solution of diffusion equations, particularly one of the variants of the Monte Carlo method.

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