

TO THE PROBLEM OF TURBULENT DIFFUSION

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1. Introduction

It's well known that mass transfer processes are realized by molecular and convection turbulent diffusion in liquids and gases. It was established experimentally that integer groups of molecules characterized by mixing lengths and turbulent viscosity participate in mixing processes of turbulent flows, contrary to the laminar streams. Turbulence favours the mixing of different impurities present in the media. Interaction of impurities leads to 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 to the 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 molecule.

2. Diffusion instability

Let molecular and turbulent diffusion take place in the medium with uniform distribution of impurity concentration $N_0(\vec{r}, t)$. They are caused by concentration gradient, 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 differentially:

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

where D and μ are molecular diffusion and mobility, respectively; \vec{V} is a medium velocity in a given point; U_0 is a volume of a unit cell; $\Pi(\vec{r} - \vec{r}')$ is the potential energy between two interacting impurities placed in \vec{r} and \vec{r}' points; $\alpha=x,y,z$, λ is an arbitrary constant parameter; $G(r,t)$ is a distribution function of impurity sources appearing or disappearing per unit of volume and per unit of time.

Using perturbation method we can write the concentration and velocity of impurity motion in the form of a sum of average and fluctuating parts:

$$N(\vec{r}, t) = N_0(\vec{r}, t) + n(\vec{r}, t), \quad N_0 \gg n; \quad \vec{V}(\vec{r}, t) = \vec{V}_0 + \vec{u}(\vec{r}, t), \quad V_0 = const \quad (2)$$

Turbulent pulsations are random function of coordinate and time with zero average mean values. The statistic of a random velocity vector field is known. Application of Picard iteration method [1] for concentration perturbation yields:

$$\begin{aligned} & [-i(\omega - \vec{k}\vec{V}_0) + Dk^2] n(\vec{k}, \omega) + \frac{\mu}{U_0} \int d\vec{k}' d\omega' \left\{ [k^2 - (\vec{k}\vec{k}')] \Pi(\vec{k} - \vec{k}') + (\vec{k}\vec{k}') \Pi(\vec{k}) \right\} N_0(\vec{k}', \omega') n(\vec{k} - \vec{k}', \omega - \omega') = \\ & = -ik_\alpha \int d\vec{k}' d\omega' N_0(\vec{k}', \omega') u_\alpha(\vec{k} - \vec{k}', \omega - \omega') \end{aligned} \quad (3)$$

In the case of solenoidal velocity field ($\vec{k} \mu_\alpha = 0$) and $N_0 = const$ we have $n(\vec{r}, t) \sim \exp(-k^2 D t)$. At $\min \Pi(k) > 0$ it is possible to introduce effective diffusion coefficient $D = D + \mu N_0 \Pi(k) / U_0$, but if $\min \Pi(k) < 0$ there exists a limiting value of impurity concentration

$$N_{0*} = - \frac{DU_0}{\mu \min \Pi(\vec{k})} \quad (4)$$

and for $N_0 > N_0^*$ negative diffusion instability arises. Generally U_0 and $\Pi(k)$ are functions of temperature T_0 and, therefore, N_0^* is a nonlinear function of T_0 . Without loss of generality let's 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 point of inflection of the function $n(x)$, i.e. $(\partial^2 n / \partial x^2)|_{x=x_0} = 0$. This is a boundary between two cells, along which the magnitude of concentration perturbation does not change. Critical value of nonexcited impurity concentration N_0 is determined by criterion of instability. At $N_0 > N_0^*$ the first cell additionally is densified at the expense of depletion of the 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 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. Consequently the analytical form of the potential energy of interacting impurity particles or clusters of different kinds of molecule plays an important role in diffusion instability evaluation.

For example, the interaction potential between Brownian particles was calculated [2] in the limit of large distance between the particles. It was shown that the particles repulse each other with a force which is inversely proportional to the cube of the distance

$$\Pi(k) = \frac{9}{8} \pi^2 R_1 R_2 k_B T_0 k^{-1} \quad (5)$$

R_1 and R_2 are radii of spherical particles, k_B is a Boltzmann constant. Using similarity method we suggest the new form of potential energy of diffusible particles

$$\Pi(k) = 4\pi(U_1 U_2)^{1/2} k_B T_0 [\cos(kR) \text{si}(kR) - \sin(kR) \text{ci}(kR)] (kR)^{-1} \quad (6)$$

R is a minimal distance of interacting clusters with U_1 and U_2 volumes; $\text{si}(x)$ and $\text{ci}(x)$ are integral sine and cosine. At small kR the curve has a form of potential hole. Increasing the parameter kR , function $\Pi(k)$ performs oscillation near zero level. At great value kR using asymptotic expansion of $\text{si}(x)$ and $\text{ci}(x)$ we obtain

$$\Pi(k) \sim -4\pi(U_1 U_2)^{1/2} k_B T_0 (kR)^{-2} \quad (7)$$

Effective potential energy of two interacting cells is negative which can account for generation of negative diffusion instability.

3. Effective diffusion coefficient

Qualitative description of impurity concentration evolution caused by molecular and turbulent diffusions has been carried out on the basis of integro-differential equation (1) and continuity equation for incompressible liquid. Using the scheme [3-5] of average field method, the closed system of equations for mean and fluctuating parts of impurity concentration has been obtained in the first order approximation

$$Q(\bar{k}, \omega) N_0(\bar{k}, \omega) + ik_\alpha \int d\bar{k}' d\omega' \langle n(\bar{k}', \omega') u_\alpha(\bar{k} - \bar{k}', \omega - \omega') \rangle = G(\bar{k}, \omega)$$

$$Q(\bar{k}, \omega) n(\bar{k}, \omega) = -ik_\beta \int d\bar{k}' d\omega' N_0(\bar{k}', \omega') u_\beta(\bar{k} - \bar{k}', \omega - \omega') \quad (8)$$

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

$$\text{where } Q(\bar{k}, \omega) = -i(\omega - \bar{k}V_0) + k^2 D + \frac{\mu}{U_0} k^2 \Pi(\bar{k})$$

The solution of system (8) yields the expression for effective diffusion coefficient:

$$D_{\text{eff}}(\bar{k}, \omega) = D + \frac{\mu}{U_0} \Pi(\bar{k}) + 2\pi \frac{k_\alpha k_\beta}{k^2} \int d\bar{k}' d\omega' W_{\alpha\beta}(\bar{k}, \Omega) = D_{\text{eff}}^{\text{mol}}(\bar{k}) + D_{\text{eff}}^{\text{urb}}(\bar{k}, \omega) \quad (9)$$

$$\text{where } \bar{k} = \bar{k} - \bar{k}', \Omega = \omega - (\bar{k}'V_0) + ik'^2 D_{\text{eff}}^{\text{mol}}(\bar{k}')$$

This formula takes into account molecular and turbulent diffusion and the interaction between impurities. Effective turbulent diffusion depends on a characteristic spatial (l) and temporal (T) scales of medium velocity pulsation, as well as on the direction of turbulent stream motion with respect to the direction of an incident radiation. This means that a turbulent diffusion coefficient becomes nonisotropic. Formula (6) is valid for arbitrary spatial-temporal tensor correlation function of homogeneous and stationary velocity field.

The expression for the transversal and longitudinal, with respect to the $\vec{\rho}_0$ vector direction ($\vec{\rho}_0 \parallel \hat{Z}$), components of turbulent diffusion coefficients in spherical coordinate system can be reduced to

$$D_{\perp}^{trb}(k_{x,y}; \omega) = 2\pi \langle u^2 \rangle \int_0^{\infty} dk' k'^4 \int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\varphi (1 - \sin^2\theta \frac{\cos^2\varphi}{\sin^2\varphi}) P(N, \Omega, l, T) \Big|_{k=k_{x,y}} \quad (10)$$

$$D_{\parallel}^{trb}(k_z; \omega) = 2\pi \langle u^2 \rangle \int_0^{\infty} dk' k'^4 \int_0^{\pi} d\theta \sin^3\theta \int_0^{2\pi} d\varphi P(N, \Omega, l, T) \Big|_{k=k_z} \quad (11)$$

where φ and θ are azimuthal and polar angles, $\langle u^2 \rangle$ is a velocity dispersion. The function $P(N, \Omega, l, T)$ can be easily restored if explicit analytical form of correlation function is known. In case of solenoidal vector field

$$W_{\alpha\beta}(\vec{N}, \Omega) = \langle u^2 \rangle (N^2 \delta_{\alpha\beta} - N_{\alpha} N_{\beta}) P(N, \Omega, l, T)$$

For instance, for diffusion correlation function taking into account the mixing of inhomogeneities with mean square root velocity $\langle u^2 \rangle^{1/2} \sim l/T$ we have [6]

$$W_{\alpha\beta}(\vec{\rho}, \tau) = \langle u^2 \rangle \left[\left(1 - \frac{\rho^2}{l_i^2} \right) \delta_{\alpha\beta} + \frac{\rho_{\alpha} \rho_{\beta}}{l_i^2} \right] M^{3/2}(\tau) \exp\left(-\frac{\rho^2}{l_i^2}\right) \quad (12)$$

where

$$l_i^2 = l^2 M^{-1}(\tau) = l^2 \left(1 + \frac{\tau^2}{T^2} \right), \quad P(N, \Omega, l, T) = \frac{\pi^2 T l^2}{2 |\vec{N}|^3} \left[1 + \frac{1}{2} (Nl)^2 - 2 \frac{(\Omega T)^2}{(Nl)^2} \right] \exp\left[-\frac{(Nl)^2}{4} - \frac{(\Omega T)^2}{(Nl)^2} \right] \quad (13)$$

4. Distribution of the mean concentration

Now we propose the new approximation of impurity concentration spatial distribution. Let a temporal horizontal component of wind velocity be located in YOZ plane. Using Picard's method the equation (1) can be rewritten in the following form:

$$\begin{aligned} \frac{\partial N^{(0)}}{\partial t} + V_y(t) \frac{\partial N^{(0)}}{\partial y} + V_z(t) \frac{\partial N^{(0)}}{\partial z} - D_{\perp} \left(\frac{\partial^2 N^{(0)}}{\partial x^2} + \frac{\partial^2 N^{(0)}}{\partial y^2} \right) - D_{\parallel} \frac{\partial^2 N^{(0)}}{\partial z^2} = \\ = \frac{\mu}{U_0} \Delta \int d\vec{r}' \Pi(\vec{r} - \vec{r}') N^{(0)}(\vec{r}', t) + G(\vec{r}, t) \end{aligned} \quad (14)$$

where D_{\perp} and D_{\parallel} are vertical and horizontal coefficients of molecular diffusion. The solution of equation (14) satisfies zero-order initial condition and boundary condition $N^{(0)}(\vec{r}) \rightarrow 0$ at $|y| \rightarrow \infty$ and $x \rightarrow \infty$ is:

$$N^{(0)}(\vec{k}, t) = \int_t^{t_0} d\tau G(\vec{k}, \tau) \exp\left[\int_{t_0}^{\tau} dt' \Omega(\vec{k}, t') \right] \quad (15)$$

$$\Omega(\vec{k}, t) = i[k_y V_y(t) + k_z V_z(t)] + [k_{\perp}^2 D_{\perp} + k_{\parallel}^2 D_{\parallel}] + \frac{\mu}{U_0} k^2 \Pi(k), \quad k_{\perp}^2 = k_x^2 + k_y^2$$

Using (2) and averaging over all possible realization of the random value $\zeta(t)$ we get

$$N_0(\bar{k}, t) = \int_0^t ds G(\bar{k}, t-s) \chi_{\zeta_y, \zeta_z}(k_y, k_z; t-s, t) \exp \left\{ -i(k_y V_{0y} + k_z V_{0z})s - \left[k_{\perp}^2 D_{\perp} + k_{\parallel}^2 D_{\parallel} + \frac{\mu}{U_0} k^2 \Pi(k) \right] s \right\} \quad (16)$$

$$\chi_{\zeta_1, \zeta_2}(k_1, k_2; t-s, t) = \exp \left[i \{ m_1 k_1 + m_2 k_2 \} - \frac{1}{2} (b_{11} k_1^2 + 2b_{12} k_1 k_2 + b_{22} k_2^2) \right] - \text{two-dimensional}$$

characteristic function of normally distributed random values [7].

$$b_{ij} = \langle \zeta_i \zeta_j \rangle = \sigma_i \sigma_j \int_0^t dt_1 \int_0^t dt_2 W(0, |t_1 - t_2|); \quad b_{ii} = \langle \zeta_i^2 \rangle = \sigma_i^2 \quad \text{and } m_i \text{ are dispersion and mean value,}$$

respectively. If $b_{12}=0$, two Gaussian random values are statistically independent. $W(\tau)$ is an arbitrary temporal correlation function. Within the scope of this theory concentration fluctuations are caused by velocity pulsations. Here we have not necessarily assumed incompressibility or isotropy. Knowledge of all parameters of fluctuating media and distribution of the mean concentration of impurities allow us to restore the characteristic size of diffusible particles.

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