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Dissipative Approach to the Calculation of the Diffusion Coefficient of the Aerosol in Turbulent Flows

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The objective of this work is to offer the methods which can be useful for calculating the coefficients of turbulent diffusion used in engineering methods of designing the chemical apparatuses for aerosol separation. The general relations for calculating the efficiency of purification process have been submitted. The offered technique is based on the dissipative approach. The results of mathematical modeling and natural experiments have been presented. A satisfactory agreement of the results of calculations according to submitted methods with experimental data has been obtained.

1. Introduction

The hydrodynamic structure of gas flow is one of the main factors determining the efficiency of aerosol particles collection in chemical apparatuses (Vincent, 1995). At the same time the flow structure is a macroscopic factor (Lohmann and Feichter, 2005) and at the micro-scale level the order of gas flow turbulence is a dominant factor which determines the mentioned efficiency (Cichocki and Felderfoh, 1991). It is especially true regarding the apparatuses with intensive regimes of phases interaction (Hewitt and Hall-Teylor, 1970).

The chaotic pulsations of the turbulent flow induce certain pulsations of flying particles with some delay depending on the particles inertness (Cichocki and Feldernof, 1991). Such character of interaction between particles and turbulent flow can be evaluated with the help of so called index of inertness $\omega\tau_r$ (Silva et al., 2011), where ω is a frequency of gas pulsations and τ_r is the relaxation time (Winkler, 1973). Provided the inequality $\omega\tau_r << 1$ is fulfilled, the relative velocity of a fine particle is about zero and the particle can be captured by the gas flow (Brener and Balabekov, 1998). And, vice versa, provided the inequality $\omega\tau_r >> 1$ is fulfilled, the particle reacts to the gas pulsations with large delay (Mednikov, 1981). This phenomenon was confirmed also with the help of numerical experiment (Khosravi and Ehsani, 2008). The prevailing role of turbulent diffusion in intensive gas flow regimes is well established. It can surpass the intensity of molecular diffusion in several times (Batchelor, 1977). The intensive turbulence of the continuum stream secures, as a rule, a constant concentration of particles having the inertness index $\omega\tau_r << 1$ nearby the surface of sedimentation (Clough, 1973). It occurs at the scale of pulsations $l > l_0$, where l_0 is the scale of micro-vortices in which the energy dissipates owing to the viscosity of medium (Davis, 1997). So, mainly the high-disperse and fine fractions of the poly-disperse aerosol are involved in the particle-laden stream (Levin and Cotton, 2009). The coarse fractions, which consist of particles with big inertness indexes, migrate owing to aerodynamic and gravity forces (Laureta et al., 2014). Thus aerosol particles are subjected to influence of turbulent pulsations with spectrum of scales from l_i to $l \sim b$ where l_i is a micro-scale of turbulence and b is a typical size of a streamlined body (Bird et al., 2007).

Thus the idea to determine the coefficient of turbulent diffusion with the help of the energy which dissipates in micro-scale pulsations of the continuum flow seems to be useful for engineering practice. Indeed this

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energy is linked with such the macroscopic characteristics as pressure drop and Reynolds number of gas flow (Kirsch and Chechuev, 1985). It opens the possibility for creating the semi-empiric technique for calculating the intensity of aerosol sedimentation in chemical apparatuses with intensive regimes of phases interaction (Li and Ahmadi, 1992). The objective of this work is to offer the methods which can be useful for calculating the coefficients of turbulent diffusion used in engineering methods of designing the chemical apparatuses for aerosol separation.

2. Governing equations

In general case the equation for calculating the evolution of aerosol particles concentration with allowing for sedimentation on elements of irrigated surfaces reads (Bird et al., 2007)

$$\frac{\partial n}{\partial \tau} + \nabla\left(J_{gen}\right) = n(r,t) \tag{1}$$

Here $n(r,t)$ is a function of particles distribution by sizes.

J_{gen} is the general stream of particles per unit of the surface of sedimentation, induced by molecular and turbulent transfer mechanisms (Bird et al., 2007):

$$J_{gen} = (D_m + D_T)\nabla n = D_{ef}\nabla n \tag{2}$$

where D_m is the coefficient of molecular diffusion, D_T is the coefficient of turbulent diffusion, D_{ef} is the effective diffusion coefficient.

The coefficient of molecular diffusion reads (Bird et al., 2007)

$$D_m = \frac{k_B T}{3\pi \nu_g d_p} \tag{3}$$

Here k_B is the Boltsman constant, T is the temperature, ν_g is the gas viscousity, d_p is the particle diameter.

Value of the coefficient of turbulent diffusion can be written as follows (Mednikov, 1981)

$$D_T = \mu^2 D_c \tag{4}$$

where D_c is the coefficient of turbulent diffusion into bulk of continuum phase, and μ is the special parameter describing the aerosol particles capture by the turbulent pulsation.

The capturing parameter can be calculated with the help of the following formula (Mednikov, 1981)

$$\mu = \sqrt{\frac{1}{1+\omega\tau_r}} \tag{5}$$

For the main stream the frequency of turbulent pulsations ω is proportional to the typical velocity of pulsations u' (Yu et al., 1998)

$$\omega = \lambda u' \tag{6}$$

Here $\lambda = 2\pi/l$ is a wave number.

Multiplying the appropriate frequency of pulsations by the square of the magnitude of turbulent pulsations we obtain the sought diffusion coefficient

$$D_c = \omega l^2 \tag{7}$$

As it follows from Kolmogoroff-Obukhov law (Kolmogorov, 1991) the velocity of turbulent pulsations can be written as

$$u' = BE^{1/3} l^{1/3} \tag{8}$$

where B is the special coefficient, and E is the energy of dissipation.
Thus Eq(4) can be rewritten as follows

$$D_c = 2\pi\gamma B E^{1/3} l^{4/3} \tag{9}$$

where γ is the correction empirical coefficient.

Then we assume that rate of the energy of dissipation is proportional to relation of the power of single turbulent vertex P_v to its mass m_v (Hanna et al., 1982):

$$E = P_v / m_v \tag{10}$$

Here the vertex power and the vertex mass can be linked with macroscopic parameters and evaluated by the formulas

$$P_v = \varphi S \frac{\rho_g u_g^3}{2} \tag{11}$$

$$m_v = V_v \rho_g \tag{12}$$

where φ is the coefficient of hydrodynamic resistance, S is a cross-section of the streamlined body or of a canal, V_v is a volume of the typical vertex, ρ_g is the gas density.

Taking into account that the size of large-scale pulsations is proportional to the diameter of the largest vertex arising into the flow, i.e. $l \sim d_v$, relation (4) can be transformed to the form

$$D_m = A\gamma\left(\frac{\varphi b u_g}{1+\omega\tau_r}\right) \tag{13}$$

3. Mass transfer into turbulent aerosol stream

The hydrodynamic analogy between friction and mass transfer is often successfully used for describing the mass transfer in turbulent flows (Kulkami and Biswas, 2004). The simplified form of the intercommunication relation between mass transfer coefficient and friction reads (Mednikov, 1981)

$$St = \frac{\beta_n}{u_p} = \frac{\lambda_{fr}}{8} Sc^{1/3} \tag{14}$$

Here β_n is the mass transfer coefficient, u_p is the particle velocity, λ_{fr} is the friction coefficient, $Sc = \nu_g / D_n$ is the Schmidt number, St is the Stanton number.

Analyzing the known methods for calculating mass transfer intensity in various systems we can conclude that used correlations are practically the same as correlations for the friction coefficient (Bird et al., 2007). So, let us suppose $\beta_n \sim \varphi$. The appropriate relation for calculating the coefficient φ reads (Bird et al., 2007)

$$\varphi = \frac{24}{\mathrm{Re}}\left(1 + \frac{\mathrm{Re}^{0.72}}{8}\right) \tag{15}$$

where $\mathrm{Re} = u_p d_p / \nu_g$.

Formula (15) is correct for $0.1 < \mathrm{Re} < 1000$.

Thus, as the main result following from (13), (14) and (15) we obtain the relation for the Sherwood number

$$Sh = \frac{\beta_n l}{D_n} = 8\left(0.375 + \mathrm{Re}^{0.72}\right) Sc^{1/3} \tag{16}$$

There are a lot of works devoted to the influence of physical-chemical properties of interacting phases on heat and mass transfer in packing columns. Analysis of the known works allows concluding that general form of the appropriate correlations can be written as following (Bird et al., 2007)

$$Sh = B\,\mathrm{Re}^{m_1}\, We^{m_2}\, Sc^{m_3} \tag{17}$$

where $We = \rho l v^2 / \sigma$ is the Weber number, σ is surface tension.

In particular, for the mass transfer in gas phase the Sherwood number can be calculated from the formula, which is correct for $\mathrm{Re} < 100$ (Mednikov, 1981)

$$Sh = 2\,\mathrm{Re}^{1/2}\, Sc^{1/3} \tag{18}$$

The influence of the Weber number on mass transfer intensity becomes significant for rather coarse droplets, i.e. for $\mathrm{Re} > 100$.

Experimental examination of relation (16) was carried out for the process of coagulation-condensation coarsening of phosphoric acid aerosols in columns with regular packing (Golubev and Brener, 2002). As turbulence inducing elements the cylindrical bodies of the diameter $b = 0.025$ m were used. These elements were placed into the contact zone of the apparatus with horizontal step $t_h = 2b$ and with different vertical steps $t_v = (1 \div 7)b$.

Figure 1 depicts some results of the experiments. From the obtained results it can be concluded that the mass transfer coefficient under vapour condensation on surfaces of aerosol particles increases practically proportional to the gas velocity. The dependence of the mass transfer coefficient on the vertical step (Figure 1) of packing units which are conducive to the turbulent pulsations is fully analogous to the dependence of hydrodynamic resistance (Brener and Balabekov, 1998). Experiments also show that the mass transfer intensity is determined by the order of turbulence of the vapour-gas flow.

This conclusion confirms the qualitative adequateness of the submitted models. Indeed the maximums of the mass transfer intensity correspond to regimes when spontaneous origins and disruptions of turbulent vertices are observed (Brener and Balabekov, 1998). The adequateness of Eqs(13) and (16) for the investigated regimes and constructive parameters is rather sufficient, of order 8%. We hardly could have got the more impressive results as the studied process was accompanied by the phase transition what complicated the analysis (Golubev et al., 2002).

The results obtained were generalized in the form of engineering expressions for calculating the efficiency of aerosol particles capturing in the irrigated apparatuses with regular packings. The appropriate relation for calculating the efficiency of inertial sedimentation on the packing elements reads

$$\eta_{in} = 1 - \exp\left(-0.75\varphi \left(\frac{\rho_l}{\rho_g} \right)^{1/3} \frac{E^{1/3} h q \Phi^2}{d_p^{1/3} u_p} \right) \tag{19}$$

Here q is specific rate of liquid irrigation, ρ_l is liquid density and ρ_g is gas density, d_p is the average droplet diameter, Φ is the droplet shape coefficient.

Due to the fine sizes of droplets their shape while flying in gas stream remains spherical and the factor Φ may be neglected as a rule.

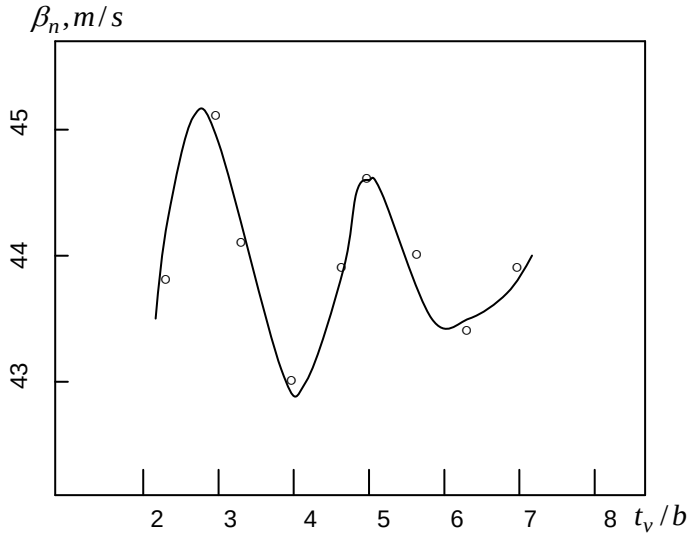

Figure 1: The dependence of mass transfer coefficient on the dimensionless vertical step between turbulence induced units. Gas velocity $W_g = 15$ *m/s; horizontal step* $t_h = 2b$

The efficiency of the diffusion sedimentation η_D can be calculated by the well-known methods (Vincent, 1995) with the help of the obtained in this paper coefficient of turbulent diffusion (13). Indeed, the efficiency of the diffusion sedimentation is a function of the Peclet number $Pe = u_g b / D_T$.

Thus the total efficiency of the sedimentation of aerosol particles in irrigated apparatuses can be obtained as follows

$$\eta_{gen} = 1 - (1 - \eta_{in})(1 - \eta_D) \tag{20}$$

Calculations which were carried out according to submitted methods while comparing with experimental data gave an error of order 12 %. Such evaluation is quite sufficient for obtaining the main constructive parameters for designing the apparatuses.

4. Conclusions

It can be concluded that the dissipative approach allowed obtaining the rather simple expressions for evaluating the effective coefficient of turbulent diffusion for fine particles in gas flows. The submitted expressions can be applied to engineering calculations of industrial apparatuses used for sedimentation of fine aerosols and gas purification. On the base of the model the relation for calculating the efficiency of inertial sedimentation on the packing elements and the relations for calculating the total efficiency of the sedimentation of aerosol particles in irrigated apparatuses have been presented. The results of the investigations are likely to be useful for calculating the intensity of mass transfer processes in chemical apparatuses and for purposes of optimal design.

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