Applied Mathematical Sciences, Vol. 10, 2016, no. 24, 1151 - 1161
HIKARI Ltd, www.m-hikari.com
http://dx.doi.org/10.12988/ams.2016.6137

Identification of Models of Transfer Processes in Complex Disperse Systems

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Abstract

Specification of model representations of complex transfer processes in liquid emulsions based on mechanisms of the basic physical phenomena (MBPP) is considered in this paper. For the representation of the complex models of the transfer processes in a generalized form a correspondence of dimensionless similarity criteria and the most simple, basic physical phenomena are used. With a lack of complete mathematical models they are replaced by a set of such basic phenomena which express physical content of a complex process. Regressive relationships between the corresponding similarity criteria are evaluated on the basis of the experimental measurement data. As a result, a formal statistical analysis is filled with an objective physical content in accordance with the nature of the MBPP.

Keywords: transfer processes, turbulent flow, liquid emulsion, basic physical phenomena, droplets breakup, fragmentation mode

1. Introduction

General physical laws of momentum, heat and mass transfer predetermine conditions of existence and character of functional dependencies of various mechanisms of these processes. A variety of mechanisms of the basic physical phenomena (MBPP), which form the complex physical processes in unstable emulsions, complicates a specification of the general mathematical models and interpretation of the results. The lack of theoretical models also complicates the analysis of empirical data and identification of the mechanisms of complex physical phenomena [1, 2].

The MBPP-interrelation, represented by the relevant dimensionless criteria, is a consequence of the differential equations structure, of the character of their exact solutions. A theoretical model of real phenomena in a full physical formula does not always give exact solutions. In this regard the model parameters remain, which must be evaluated, taking into account a variety of conditions and specific technological processes that use them. In such cases the dependency in the criterial form can be obtained only on the empirical basis for statistical analyses of experimental data.

However even incomplete theoretical representations are important for understanding the structure of the complex physical processes. They help prove the composition of the MBPP and specify empirical models, using corresponding dimensionless similarity criteria. These hypothetical model approximations are checked and made more precisely by the statistical analysis of the relevant experimental data. Adequate specifications of composition of the basic physical mechanisms, represented by the experimental data, in turn, contribute to understanding the character of the studied phenomena.

2. Presentation of complex physical phenomena by mechanisms of elementary transfer processes

When developing a generalized dependence, the MBPP is included in the form of dimensionless criteria that correspond to them on the basis of prior theoretical and empirical physical concepts. For a substantiation and a more precise definition of prior beliefs about the character of their physical transfer processes, statistical values of the model parameters and the quality of the approximation of empirical data are used.

2.1. Elementary transfer processes when moving viscous fluid through pipelines

Let us consider a simple illustrative example of how the mechanisms of the basic physical phenomena are identified and used. A model of flow of a viscous incompressible fluid in a pipe with a circular cross-section under the laminar regime is represented by a differential equation of motion:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dU(r)}{dr}\right)=-\frac{1}{\mu}\frac{\Delta p}{L} \tag{1}$$

with a boundary condition of sticking to the tube wall with R radius

$$U(r) = 0 \text{ at } r = R. \quad (2)$$

Integrating of the equation (1) with a boundary condition (2) gives an exact particular solution to the problem. Velocity distribution in a stream of fluid across the section of the circular pipe with a diameter $D = 2R$ and length L is:

$$U(r) = -\frac{1}{\mu}\frac{\Delta p}{L}\frac{(r^2 - R^2)}{4}. \quad (3)$$

The detailed dependence of (3) does not contain all hydrodynamic characteristics. Turning to the averaged representation of the exact solution using the average flow rate Q of the flow velocity U we get:

$$Q = \overline{U}\pi R^2 = \int_0^R 2\pi r U(r)dr = -\frac{1}{\mu}\frac{\Delta p}{L}\frac{\pi R^4}{8}.$$

The exact solution of the problem (1) in a more general form of the criterion is:

$$Eu = \frac{32}{Re}\frac{L}{D}, \quad (4)$$

where the dimensionless criteria of similarity are: $Re = \rho\overline{U}D/\mu$ - the Reynolds number, $Eu = \Delta p/(\rho\overline{U}^2)$ - the Euler's number.

It is clear that these criteria determine the character of physical phenomena, formalized by the model theoretical representation (1)-(2). It was found that the flow of a viscous fluid is connected with two dimensionless criteria. The number *Re* defines the laminar motion regime while the internal friction of fluid depends only on its dynamic viscosity μ. And the number *Eu* represents a drive force of a pressure flow due to the pressure drop Δp. Therefore, criterial dependence (4) can be interpreted as a relationship of the basic mechanisms of the transfer processes, which are represented in the pressure flow of a viscous fluid in laminar flow. It should be noted that we can get them by writing the equation of motion (1) in a dimensionless form.

Let us consider an opposite hypothetical situation, when a formulation of a desired theoretical model is not possible. However there is the evidence of experimental studies on the basis of which it is desirable to obtain a calculated dependence, similar to the previously obtained criteria dependence (4). In such a way due to the research of the blood movement through the capillary vessels, physiologist J. Poiseuille established the following facts, published in 1840 in the reports of the Paris Academy of Sciences:

a) when a steady laminar motion of viscous incompressible fluid in a pipe of circular section the volumetric flow rate Q is proportional to the pressure drop Δp per unit of a pipe with length L,

b) volumetric flow rate Q is proportional to the fourth power of its radius (diameter).

From the general physical representations of possible mechanisms of the basic physical transfer processes follows a hypothesis, that under these circumstances there may be only two determinant criteria: *Eu* and *Re*. The estimated functional relationship between them can be described in general as follows:

$$Eu = C\,Re^{\alpha}\,, \tag{5}$$

where the constants C and α are determined on the basis of the previously accepted empirical Poiseuille facts a) and b).

Let us represent the formula (5) with the accuracy up to the constants in the form, which contains all the dimensional variables, measured by Poiseuille (additional multiplier D^{β} is needed to consider the second experimental fact):

$$\frac{\Delta p}{L}\frac{D^4}{\rho Q^2} = C\left(\frac{\rho Q D}{\mu D^2}\right)^{\alpha} D^{\beta}\,.$$

From a comparison of the degrees of $\Delta p/L$ and Q we get a ratio: $1 = 2 + \alpha$, $\alpha = -1$. Similarly, for degrees Q and D follows: $4 + \alpha - \beta = 4(2 + \alpha)$, $\beta = 4$. As a result, after transformation we get the criteria dependence analogous to (4) based only on the experimental facts:

$$Eu = \frac{C}{Re}\frac{L}{D}\,. \tag{6}$$

Therefore, the Poiseuille experimental facts turned out to be equivalent to the mathematical model (1), physical content of which was interpreted by the elementary mechanisms of transfer processes. However, for the constant C evaluation, quantitative data of experimental studies are needed. Since the flow in pipes of circular cross-section is well understood, the results of numerous measurements are systematized in the form of the coefficient of hydraulic resistance λ using the Darcy-Weisbach formula:

$$\Delta p = \lambda \frac{L}{D}\frac{\rho \bar{U}^2}{2}\,. \tag{7}$$

For the laminar fluid flow regime when Re < 2320, the formula $\lambda = 64/Re$ corresponds to the experimental data. Comparison of the expressions (6) and (7) gives the constant $C = 32$, which provides a full correspondence with the criterial form of the exact solution (4).

Without the exact solution (4), stability of the values of the constant C means the lack of a significant effect of other mechanisms of the basic transfer processes. Such a conclusion is made on evaluating the constant using real empirical data, when the variance estimation is within the limits of random errors of measurement. However, if the dimensionless model (5) is formulated on the basis of inadequate physical representations, it is not acceptable.

Thus, if $Re > 10000$, when the flow is turbulent, the basic mechanisms of transfer processes are related to the fundamentally different, whirling motion. The change of the general physical conditions leads to the other model representations, which cannot correspond to the theoretical equation of motion (1). Therefore, the dimensionless equation (4) becomes invalid. Principal changes are reflected by the coefficient of hydraulic resistance, which is determined by the empirical Blasius formula $\lambda = 0.3164/Re^{0.25}$. Comparison of the expressions (6) and (7) gives in this case $C = 0.16/Re^{0.75}$, suggesting an inadequacy of the model (4) to character of physical processes, which were represented by the data of the experiments. The inadequacy can be eliminated by an additional basic mechanism of turbulent transfer that satisfies the empirical factor $Re^{0.75}$.

2.2. Elementary transfer processes during droplets breakup in a homogeneous turbulent flow of emulsion

As a more complex example the deformation and droplets breakup of a viscous fluid are considered under the influence of dynamic and shear stress in a turbulent flow. Until today this task remains quite challenging for a theoretical analysis. Therefore, numerous empirical correlations for the calculation of the maximum stable diameter of droplets are often formal. By means of the basic transfer processes the analysis of empirical data makes it possible to identify the mechanisms of the complex physical phenomena in the luck of their theoretical models.

Unlike the homogeneous fluid, the number of criteria for emulsion, representing the MBPP, is much greater, in accordance with the number of the dimensional variables. Therefore, the selection of the MBPP and functional relationships between them are determined by the existing physical ideas about the character of interaction between dispersed droplets with the turbulent emulsion flow.

The main dimensionless criterion, representing the basic processes of the droplets breakup in a turbulent flow, is the Weber number *We*. The criterion is the ratio of the surface energy $E_\sigma = d/\sigma$, which ensures the integrity of the droplets, and the destabilizing external force energy *E*. Taking into account the hypothesis of the universality of the dimensionless local structure of a turbulent flow, A.N. Kolmogorov defined the microscale of a turbulent fluctuations λ_0 [3]. At the distances *d* exceeding the microscale, the vortex motion of fluid becomes inertial. The magnitude of the averaged squared difference of the velocity fluctuation is determined only by the consumption of energy in unit of mass per unit of time ε:

$$\bar{v}^2 = C_1(\varepsilon \cdot d)^{2/3} \tag{8}$$

Thus, the diameter of the maximum stable droplets depends on the inertial forces energy resulting from the turbulent speed fluctuations $E = \rho_c \bar{v}^2$. These forces are caused by the fluctuations change at distances comparable to the diameter of the droplets. Kinetic energy of the turbulent fluctuations increases with the increase in their size. In case the droplets breakup is carried out by the fluctuations, dynamic mechanism the Weber number is written as the ratio of the energy of the inertial and surface forces - $We = \frac{\rho_c \bar{v}^2 d}{\sigma}$.

The theoretical concepts of A.N. Kolmogorov were used by Hinze in the experimental data analysis associated with an inertial fragmentation mode [4]. It has been shown that there is a critical value of the Weber number $We^* = 0.585$, the exceedance of which leads to the droplets breakup. On the assumption of the views associated with the basic transfer processes $We = const$ means that the breakup can be associated with only one inertial mechanism. This mechanism is represented by the estimated formula for d_{max}, which is widely used until the present time:

$$d_{max} = \left(We^{*}\sigma / \rho_c\right)^{3/5} \varepsilon^{-2/5}. \tag{9}$$

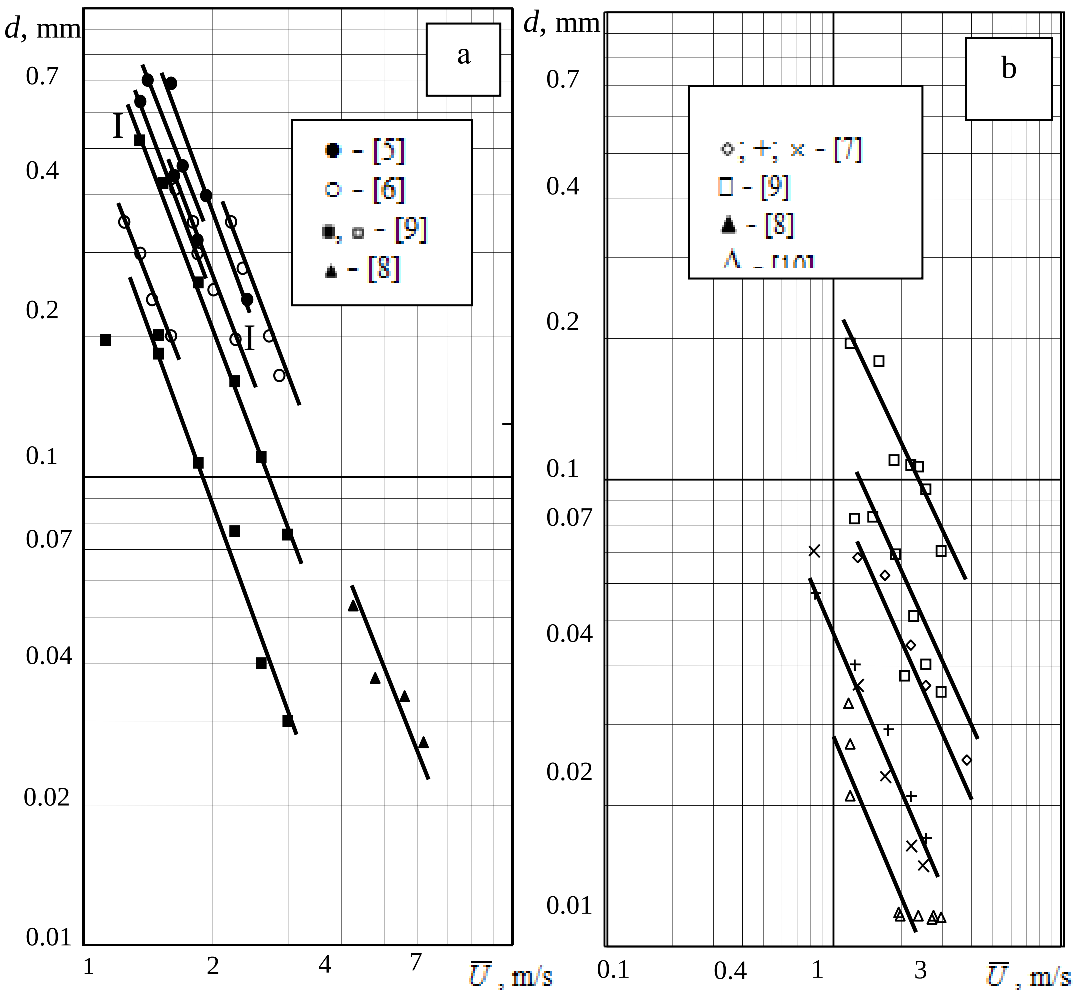

Fig.1. The character of experimental data of the droplets breakup in pipelines [11]

Droplets fragmentation mode: *a*) $d_{max} \approx \overline{U}^{\,-2,5}$, *b*) $d_{max} \approx \overline{U}^{\,-1,2}$

However, as a result of size measurements of breakup resistant droplets in a pipeline with a diameter of 0.038 m Sleicher [5] found a completely different relation on the averaged flow rate: $d_{max} \approx \overline{U}^{-2.5}$. Sleicher saw an experimental data mismatch in the unacceptability of the basic assumptions of the theory associated with an isotropic turbulent flow. Based on the analysis of the high-speed cinephotomicrography materials it was recorded that very unstable droplets always deform and break up in the wall area. Though according to Fig. 1 it can be detected by the experimental analysis of many authors, this new experimental fact remained unknown in literature. It can be explained mainly by the existing standard approach and by the lack of a serious theoretical substantiation, similar to the widely used Kolmogorov- Hinze correlation (9).

The reason of the inadequate attention for the Slecher correlation is the absence of a theoretical model representation of the deformable fluid droplets breakup in a turbulent flow. Besides, the inertial and viscous Weber criteria represent the mechanisms of the basic physical phenomena that are cross-interrelated processes.

2.3. Simulation of droplet breakup mechanisms in non-uniform turbulent flow

Based on the experimental facts about emulsion behavior under the conditions of the wall turbulence, it is natural to consider the deformation of droplets, which increases the breakup process efficiency. The viscous shear stress due to the averaged velocity gradient at the pipe walls and the inertial forces of the turbulent fluctuations are not summed over, in some way altering the structure of the general functional relationship. The form can be evaluated only on the basis of the experimental facts and inclusion of the basic breakup processes in criterion dependence on the basis of clear physical representations [11].

It is obvious that as a primary basic process, it is natural to consider the inertial droplet breakup mechanism of the dispersed phase by means of velocity fluctuations of the emulsion continuous medium. Stability of the droplets is supported by the surface stress, intensity of which is proportional to the surface curvature. During the deformation by shear stress a spherical form is changed to the oblong ellipsoid of revolution with a variable curvature. The side surface of the extended along the flow ellipsoid can greatly reduce the curvature of the original sphere. This leads to a local destabilization of the droplet, which was able to withstand the turbulent fluctuations.

For the correction of the droplets curvature changes, let us use its effective value of the diameter d_{ef}, associated with the diameter of the original sphere of the same volume of an unknown function of deformation rate: $d_{ef} = d_{max} f(F)$. A generalization of the Kolmogorov-Hinze inertial breakup mechanism is in the change of the original diameter of a droplet by an effective value, determined by the deformation through the velocity gradient at the pipeline wall:

$$\rho_c d_{ef} \bar{v}^2 / \sigma = C_2 \tag{10}$$

Under the simple shear conditions the dependence of the droplet deformation related to the magnitude of the gradient G and physical properties of liquids is obtained by Taylor [12]:

$$F = \frac{G \cdot d \cdot \mu_c}{2\sigma} \left(\frac{19\mu_d / \mu_c + 16}{16\mu_d / \mu_c + 16} \right). \tag{11}$$

As follows from the Taylor theory, when the viscous forces are high, compared to the interfacial tension forces, the droplet deforms. When the maximum deformation value is reached, the droplet loses stability and breaks up. Under the conditions of a non-uniform turbulent flow the results of this theory are mainly qualitative. However, they allow obtaining another dimensionless criterion and inherent physical characteristics.

The averaged velocity gradient taking into account the logarithmic distribution law at a distance comparable to the droplet diameter from the hydraulically smooth pipe wall can be estimated as follows:

$$G = \frac{\bar{U}(y+d) - \bar{U}(y)}{d} = \frac{u_*}{\kappa d} \left[ln \frac{(y+d)\nu_c}{u_*} - ln \frac{y \nu_c}{u_*} \right].$$

We suppose that the droplet is deformed sufficiently close to the pipe wall, and the dynamic speed $u_* = \sqrt{\lambda / 8} \cdot \bar{U}$, λ is a coefficient of hydraulic resistance. Thus, we obtain $G = \sqrt{\lambda} \cdot \bar{U} / d$ with an accuracy to constants and the Taylor expression for the deformation (2.5) can be expressed as:

$$F = \frac{\sqrt{\lambda}\, \mu_c \cdot \bar{U}}{\sigma} \cdot \varphi\left(\frac{\mu_d}{\mu_c} \right), \tag{12}$$

where the function of the viscosity ratio of the emulsion phases remains unknown.

Thus, it is proved that the breakup mechanism of the gradient corresponds to the dimensionless Weber criterion for a continuous medium, and to the Reynolds number, according to the Blasius formula: $\lambda = 0{,}3164/ Re$.

To obtain the previously unknown influence of the droplets deformation, it is necessary to use the empirical Slecher correlation $d_{max} \approx \bar{U}^{-2{,}5}$ for breakup in the non-homogeneous turbulent flow [5, 6]:

$$\rho_c d_{max} \left[\frac{\sqrt{\lambda}\mu_c \cdot \bar{U}}{\sigma} \varphi\left(\frac{\mu_d}{\mu_c} \right) \right]^{\alpha} \cdot \frac{\bar{U}^2}{\sigma} = C_2^*.$$

The equation for α is written as $\alpha + 2 = 2.5$, and hence we obtain $\alpha = 0.5$. The functional expression of the gradient mechanism included in the basic physical process of pulsation breakup takes the form $d_{ef} = d_{max} F^{0{,}5}$. It is obvious that the constant C_2^* should be approximated to the empirical function of viscosity ratio μ_d/μ_c, and its nature is studied in a simple shear field [13].

It is evident that low-viscosity droplets (or steam bubbles), the diameters of which are smaller than the microscale of turbulence λ_0, can be destroyed in accordance to another gradient-based mechanism. The smaller the scale of vortex motion is, the greater the gradients of velocity fluctuations are [14], this implies predominance of the viscous shear stress energy $E = \mu_c \overline{G}$. Under the assumption of the local isotropy, G. Batchelor received the following expression for the averaged gradient of turbulent fluctuations:

$$\overline{G} = \sqrt{2\varepsilon / 15\nu_c} \tag{13}$$

For this basic breakup process the Weber number is written as the ratio of the averaged gradient energy of the velocity fluctuations and surface forces, that prevent the droplets deformation:

$$We = \mu_c \overline{G}\ d / \sigma . \tag{14}$$

In mixing apparatus with turbine mixers the droplets breakup mechanism is implemented, when the energy of turbulence ε is high and the influence of the averaged gradient of turbulent fluctuations predominates [15].

3. Conclusion

The results of the research show that in liquid emulsions, the actual processes of the momentum and heat transfer significantly depend on the expenditure and geometric characteristics, as well as on the character of the phases interaction. This is due to the lack of the common theoretical models, reflecting the diversity of the folding mechanisms of transfer processes. The MBPP are flexible tools for shaping the model of the criterial relationships. To justify their supposed composition the dimensionless similarity criteria are used, which provide the physical content of the formal regression relationships.

The specification of the model ratios is complicated by the interrelated MBPP which not only complete, but also modify each other. In such cases the functional form of the empirical dependence is specified by the inclusion of an additional criterion to the major one. The acceptability of the approved ideas and evaluation of the model constants are based on the data of experimental studies.

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Received: February 14, 2016; Published: March 30, 2016