KAPITEL 7 / *CHAPTER 7* [7]
PECULIARITIES OF MASS TRANSFER PROCESSES DURING DILUTION OF IMPURITIES IN SINGLE-PHASE AND AERATED FLOWS

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Introduction and problem statement

The problems of viscosity have been thoroughly considered in [1-2] on the basis of the existing theory, which is closely related to the mechanics of continuum and the molecular theory of fluids. According to these theories, the concept of viscosity can be determined on the basis of the molecular structure of the fluids under consideration.

For example, in Eyring's theory, based on the theory of absolute reaction rates, the movement of molecules is considered as passing through a potential barrier, which describes the processes of chemical reaction kinetics.

In particular, based on the molecular theory of viscosity, a dependence was proposed for determining dynamic viscosity. For the molecular level, it is expressed in terms of activation energy [3-4]

$$\mu = \frac{A}{\omega(\omega - a)} \exp\left[B(\omega,T) \cdot KT^{-1}\right], \tag{1}$$

where A is a constant related to the frequency of molecular vibrations; $B(\omega,T)$ – isochoric temperature coefficient of viscosity; ω – molecular volume; T – absolute temperature; K – Boltzmann constant; a – volume of densely packed molecules.

The rheological model of most fluids in steady state motion can be represented in terms of momentum flux density. The internal friction forces between two layers of a gas or liquid are valid for the macro level. Described by Newton's law:

$$I_L = -\eta \frac{du}{dx}, \tag{2}$$

where η – coefficient of dynamic viscosity, $\frac{du}{dx}$ – the velocity gradient, which is the rate of change of velocity in the x direction, perpendicular to the direction of movement

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of the layers.

This definition of viscosity was originally proposed by Newton. This definition is, of course, microscopic, expressed in terms of quantities that cannot be measured [5-7].

Macroscopic definition of viscosity. The above methods have a common feature - they measure the work that must be spent to maintain a steady flow, that is, these methods measure the energy dispersed (dissipated) by the frictional forces inherent in a viscous flow.

The viscosity coefficient can be determined based on diffusion methods, and viscosity can be expressed using the diffusion coefficient.

Based on other theories, viscosity can be expressed by the following analytical dependence of μ on T according to the studies of G. M. Panchenkov

$$\mu = 3\sqrt{6R} \cdot \sqrt{\frac{\omega_w^2}{N_0}} \cdot \rho^{\frac{4}{3}} \cdot M^{-\frac{5}{4}} \cdot T^{\frac{1}{2}} \times e^{-\frac{\varepsilon}{R \cdot T}} \cdot \left(1 - e^{-\frac{\varepsilon}{R \cdot T}}\right)^2, \quad (3)$$

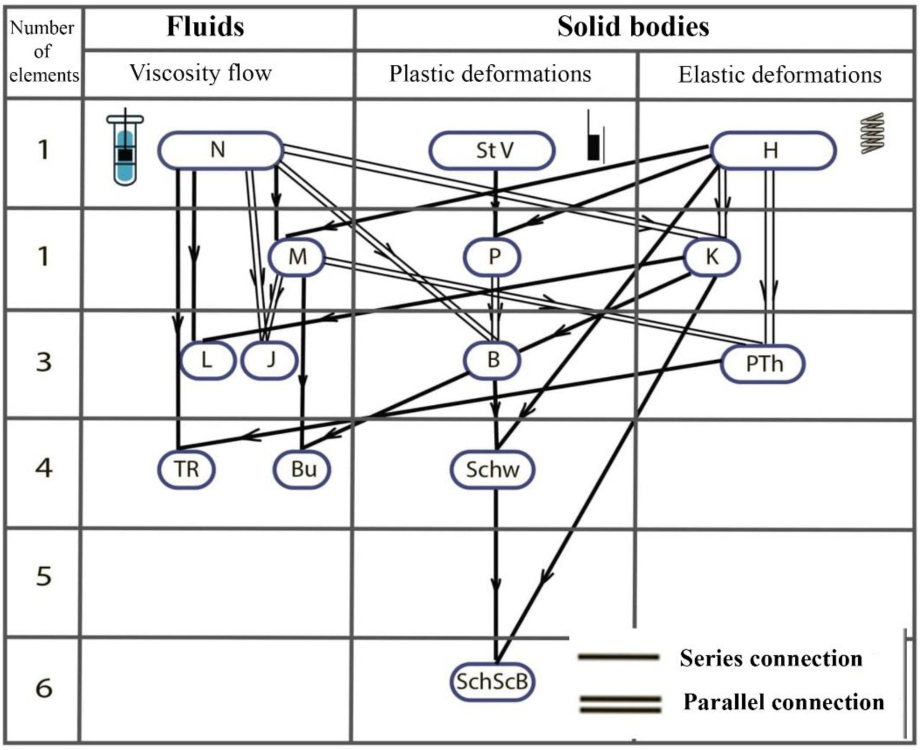
where R – gas constant; ω_w – intrinsic volume of molecules in calculations per 1g-mol; N_0 – number of molecules in 1g-mol volume; M – molecular weight; ρ – density; ε – the binding energy of the molecules of a liquid, determined by the work required to move it infinitely far from its initial position. This work is equal to the latent heat of vaporization divided by half the coordinate number of the liquid.

In many cases, taking into account the rheological complexity of various environments, which, as noted in [1, 2], can have both viscous and elastic properties. To describe rheologically complex systems, mechanical models proposed in Reiner's work [1, 2] are used. These models are based on information about the properties of environment analogies.

The set of existing rheological properties can be represented as a system consisting of ideal bodies. Of these, three bodies are represented in continuum mechanics: a solid body Hooke's law (H), a plastic body Saint-Venant (StV), and a Newtonian fluid (N). More rheologically complex bodies can be obtained by appropriate combinations of these laws in parallel or series connection, which allows to describe not only elongation and shear, but also counter-stretching. Mechanical models of macrorheology of Newtonian and, accordingly, visco-plastic or Bingham bodies of non-Newtonian fluids can be represented by the corresponding rheological system [4, 8-9].

Table 1 shows a system of rheological bodies constructed according to the structure of the elements that form the body.

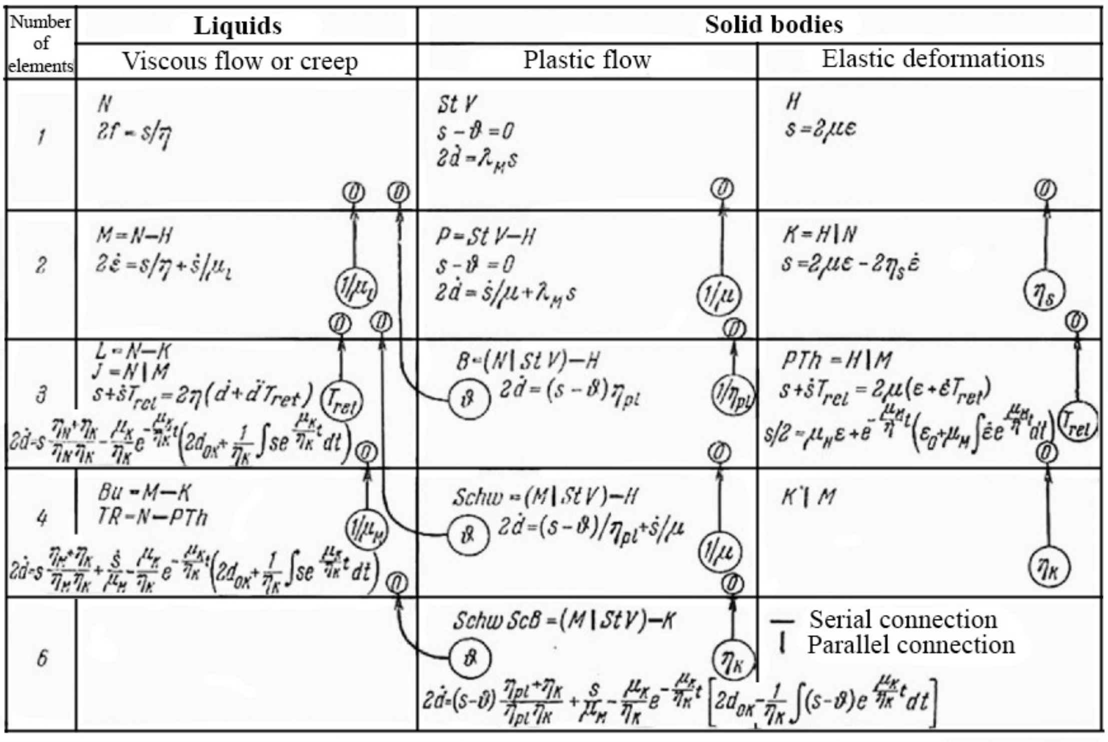
Table 1 - System of rheological bodies constructed according to the structure of elements



Based on this scheme, the considered rheological models can be described by a system of rheological equations. A description of the first-order phenomena for the viscous, elastic and plastic states of matter is given in Table 2.

As can be seen from the above table, the rheological properties of various environments, and accordingly the transport coefficients, can be described not only by the viscosity value, but also by other physical constants, such as the modulus of elasticity, plasticity, etc.

Table 2 - System of rheological equations



Number of elements	Liquids	Solid bodies	
	Viscous flow or creep	Plastic flow	Elastic deformations
1	N $2f = s/\eta$	St V $s - \vartheta = 0$ $2\dot{d} = \lambda_M s$	H $s = 2\mu\varepsilon$
2	M = N—H $2\dot{\varepsilon} = s/\eta + \dot{s}/\mu_1$	P = St V—H $s - \vartheta = 0$ $2\dot{d} = \dot{s}/\mu + \lambda_M s$	K = H|N $s = 2\mu\varepsilon - 2\eta_s\dot{\varepsilon}$
3	L = N—K J = N|M $s + \dot{s}T_{rel} = 2\eta(\dot{d} + \ddot{d}T_{ret})$ $2\dot{d} = s\frac{\eta_N + \eta_K}{\eta_N\eta_K} - \frac{\mu_K}{\eta_K}e^{-\frac{\mu_K}{\eta_K}t}\left(2d_{0K} + \frac{1}{\eta_K}\int se^{\frac{\mu_K}{\eta_K}t}dt\right)$	B = (N|St V)—H $2\dot{d} = (s - \vartheta)\eta_{pl}$	PTh = H|M $s + \dot{s}T_{rel} = 2\mu(\varepsilon + \dot{\varepsilon}T_{ret})$ $s/2 = \mu_H\varepsilon + e^{-\frac{\mu_H}{\eta}t}\left(\varepsilon_0 + \mu_M\int\dot{\varepsilon}e^{\frac{\mu_H}{\eta}t}dt\right)$
4	Bu = M—K TR = N—PTh $2\dot{d} = s\frac{\eta_M + \eta_K}{\eta_M\eta_K} + \frac{\dot{s}}{\mu_M} - \frac{\mu_K}{\eta_K}e^{-\frac{\mu_K}{\eta_K}t}\left(2d_{0K} + \frac{1}{\eta_K}\int se^{\frac{\mu_K}{\eta_K}t}dt\right)$	Schw = (M|St V)—H $2\dot{d} = (s - \vartheta)/\eta_{pl} + \dot{s}/\mu$	K'|M
6		Schw ScB = (M|St V)—K $2\dot{d} = (s - \vartheta)\frac{\eta_{pl} + \eta_K}{\eta_{pl}\eta_K} + \frac{s}{\mu_M} - \frac{\mu_K}{\eta_K}e^{-\frac{\mu_K}{\eta_K}t}\left[2d_{0K} - \frac{1}{\eta_K}\int(s - \vartheta)e^{\frac{\mu_K}{\eta_K}t}dt\right]$	— Serial connection | Parallel connection

7.1. Transfer processes and their analogy

Transport processes constitute a significant class of phenomena that occur during fluid motion. They are widely used in calculations of engineering systems, which include the transfer of momentum, impurities and heat [3-4].

In all three cases, the substance of transportation is water. Accordingly, the laws that describe the motion of this fluid, in one way or another, describe the regularities of the transfer of various substances in it. The analogy between the processes under consideration is very clear, which can be traced in turbulent motion, when the transfer of a substance occurs by individual moles of the substance.

According to Newton's hypothesis, the rate of transfer of momentum is determined from the dependence

$$\frac{\tau}{\rho} = -\epsilon_T \frac{dV}{dn}. \tag{4}$$

As mentioned, the mass transfer rate is described by Fick's first law

$$m = -D_T \frac{dC}{dn}. \qquad (5)$$

By analogy, the rate of heat transfer is characterized by Fourier's law

$$q = -E_T \frac{d(\rho C_p T)}{dn}. \qquad (6)$$

In the above formulas, the values ϵ_T, D_T, E_T calculate like this:

$\epsilon_T = \dfrac{\Delta V_x \Delta V_y}{\frac{dV}{dn}}$; $D_T = \dfrac{\Delta V_y \Delta C}{\frac{dC}{dn}}$; $E_T = \dfrac{\Delta V_y \Delta T}{\frac{dT}{dn}}$ – coefficients of turbulent viscosity, diffusion and heat transfer. Де $\Delta V_x; \Delta V_y; \Delta C$, ΔT – pulsations of velocity, concentration and temperature, averaged over time, and $\frac{dV}{dn}; \frac{dC}{dn}; \frac{dT}{dn}$ – gradients of average velocity, concentration and temperature, C_p – specific heat capacity.

It is interesting that the transfer coefficients ϵ_T; D_T; E_T have the same unit of measurement – m^2/s. In addition, they are units of the same order, that is

$$\epsilon_T \approx D_T \approx E_T. \qquad (7)$$

The analogy of the transfer of momentum, mass, and heat, as well as condition (7), were first formulated by Reynolds.

Dividing the turbulent viscosity coefficient ϵ_T on the turbulent diffusion coefficient D_T and the turbulent heat transfer coefficient E_T, we obtain the dimensionless turbulent Schmidt numbers Sc and Prandtl numbers Pr

$$\mathrm{Sc} = \frac{\epsilon_T}{D_T}; \mathrm{Pr} = \frac{\epsilon_T}{E_T}. \qquad (8)$$

According to Reynolds analogy

$$\mathrm{Sc} \approx \mathrm{Pr} \approx 1. \qquad (9)$$

The obtained condition has a deep physical meaning. It demonstrates that the profile of averaged velocities in the flow cross-section completely coincides with the profile of concentration and temperatures. In addition, the adopted condition makes it possible to use a large amount of experimental data on the study of the hydrodynamic structure of flows in treatment plants in calculations of mass and heat transfer processes

[6, 8].

Further studies have shown that a Schmidt number of $\mathrm{Sc} \approx 0,7$ is more accurate, meaning that the concentration profile will be more elongated compared to the velocity profile.

When considering processes occurring at the molecular level, the molecular Schmidt number is used.

$$Sc_M = \frac{\nu_M}{D_M}. \tag{10}$$

For gases $Sc_M \approx 1$, and for a liquid in laminar motion $Sc_M \approx 10^3$.

The motion mode is characterized by the Reynolds number

$$\mathrm{Re} = \frac{Vl}{\nu}. \tag{11}$$

A similar combination for diffusion is given by the Peclet number

$$\mathrm{Pe} = \frac{Vl}{D}. \tag{12}$$

In the case when $\mathrm{Pe} << 1$, the mass transfer process occurs due to molecular diffusion, and when $\mathrm{Pe} >> 1$ – due to turbulent diffusion.

Dilution of impurities in single-phase flows

An example of this mass transfer process is the dilution of wastewater in an open flow, where the transfer of passive impurities occurs due to turbulent diffusion and non-uniformity of the average velocity distribution in the flow cross section. For the analysis, we will use Fick's second law [8-9].

Considering steady motion $\left(\frac{dC}{dt} = 0\right)$, and also accepting $V_x = V; D_y = D_T; V_y = 0;$ $V_z = 0; D_x = 0; D_z = 0.$, we get the equation

$$V\frac{dC}{dx} = D_T\frac{d^2C}{dy^2}. \tag{13}$$

The resulting equation is calculated using computer technology.

In particular, according to the solution proposed by V. V. Smyslov, dependence

(13) is presented in the form

$$\frac{dC}{dx} = y_* \frac{d^2C}{dy^2}, \tag{14}$$

where y_* is called the linear parameter of turbulent diffusion and is calculated

$$y_* = \psi H \sqrt{\frac{gH}{W}}, \tag{15}$$

where W – speed characteristic, ψ – experimental coefficient.

$$\psi = 0{,}25 + 2{,}8(\phi - 1).$$

Here the meaning $\phi = \dfrac{l}{l_n}$ – meandering of the riverbed (l, l_n – the length of the river from the place of discharge of passive impurities to the calculated alignment along the fairway and along the straight line). For a straight channel $\phi = 1$ i $\psi = 0.25$.

Having solved equation (14), we obtained a formula for determining the relative maximum concentration of impurities at a length l from the discharge point

$$\vec{C}_м = \frac{0{,}28B}{\sqrt{y_* l}}, \tag{16}$$

where B – width of the riverbed.

A formulaic decision is considered fair if

$$\frac{B}{\sqrt{y_* l}} = 350...20. \tag{17}$$

Using the relation, it should be assumed that the initial impurity concentration here is taken as $C_n = 100$, and then $\vec{C}_м = C_м/100$. Where is the value $C_м$ expresses the maximum concentration relative to the initial one. In the case where the initial concentration is given in milligrams per liter (mg/L), then the maximum concentration at this point will be in mg/L.

$$C_м = C_n \frac{\vec{C}_м}{100}. \tag{18}$$

Given the geometric and hydraulic parameters of the channel B, H, ϕ and the given concentration C_n impurities, using equations you can get the maximum concentration value $C_м$ in any alignment at a distance l within the limits given in the relation.

The process of mixing passive impurities with water in a watercourse is characterized by the dilution factor n, which is calculated as follows:

$$n = \frac{C_{cm} - C_p}{C_{\max} - C_p}, \text{ or } \quad n = 1 - \frac{1 - e^{-K\phi\sqrt[3]{\frac{D_T}{q}l}}}{1 + e^{-K\phi\sqrt[3]{\frac{D_T}{q}l}}\frac{Q}{q}}, \qquad (19)$$

where C_{cm}, C_p – concentration of impurities of one type in wastewater and in a water body up to the point of wastewater discharge, C_{max} – maximum possible concentration of impurities in the design section of a water body, Q, q – River and wastewater flow (m^3/s), D_T – turbulent diffusion coefficient, K – coefficient that depends on the location of the wastewater discharge in the watercourse. When discharged near the shore $K = 1$, and on the axis of the river $K = 1,5$.

The distance to the design point (m), in which dilution with a given multiplicity is ensured, is calculated according to the dependence

$$l = \frac{q}{D_T}\left(\frac{1}{K\phi}l.n\frac{n\frac{Q}{q}}{1 + \frac{Q}{q} - n}\right)^3. \qquad (20)$$

7.2. Features of the mass transfer process in aerated flows

These processes occur in wastewater treatment plants during the process of supplying air to the liquid being purified. Air is supplied to the water in the form of bubbles with a diameter of $d_б \approx 3...8mm.$ When they come into contact with water, oxygen from the bubbles passes into the water, ensuring the vital activity of microorganisms in the treatment plants.

The mass transfer rate for such processes is described by Fick's first law. Due to the complexity of its definition, Fick's first law is usually written in the form

$$m=\frac{D_{еф}}{n}(C_S-C)=\beta(C_S-C)\,, \qquad (21)$$

where n – film thickness at the interface between air and water in bubbles, C_S – saturation concentration of a liquid with gas (solubility in water at a given concentration in air), C – concentration of oxygen transition mass in water, $\beta=\frac{D_{еф}}{n}$ – mass transfer coefficient, which is determined experimentally, for each type of treatment plant.

In some cases, the value of β is estimated analytically. For example, for bubbles with a size of β, when the flow is laminar and mass transfer is mainly due to molecular diffusion, the value of $d_б < 3мм$ is calculated as follows

$$\beta=2\sqrt{\frac{D_M}{\pi.t}}=2\sqrt{\frac{D_M V_б}{\pi.d_б}}\,, \qquad (22)$$

where $t=\frac{d_б}{V_б}$ – the time the liquid volume element remains at the phase multiplication boundary "exposure time", $V_б$ – The rate at which the bubble rises to the air (fig. 1) is found from the graph.

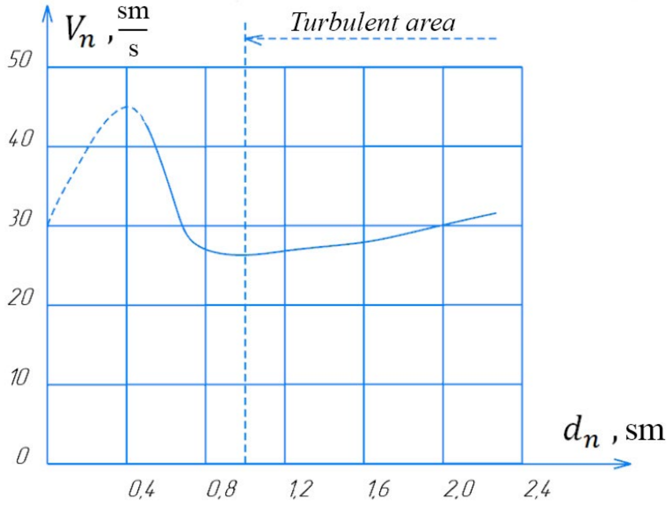


Fig. 1. The rate of bubble rising to air

For larger bubbles ($d_б$ >mm), the hydrodynamic situation near the interface is significantly complicated by flow turbulence. In this case, the mass transfer coefficient will depend only on the averaged exposure time

$$\beta = \sqrt{D_{еф} S}\,, \tag{23}$$

where S – the frequency of updating the phase contact surface, which for the turbulent flow regime is determined by the magnitude and intensity of the pulsation and calculated from experimental data.

The resulting formulas are indicative in nature. The value of β is significantly affected by the presence of various impurities, in addition, the speed of bubbles will be a variable value. Therefore, the most reliable way to determine β is a method based on the use of experimental results or data obtained during the operation of treatment plants.

Summary and conclusions

Based on the conducted research, the features of mass transfer processes during the dilution of impurities in single-phase and aerated flows were analyzed. The corresponding dependences for the dilution of wastewater in an open flow were obtained, where the transfer of passive impurities occurs due to turbulent diffusion and uneven distribution of average velocities in the flow cross section. The processes occurring in wastewater treatment plants when air is supplied to the liquid being cleaned were investigated.