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Mathematical Model For Measuring The Concentration Of Particles In A Liquid During Their Sedimentation

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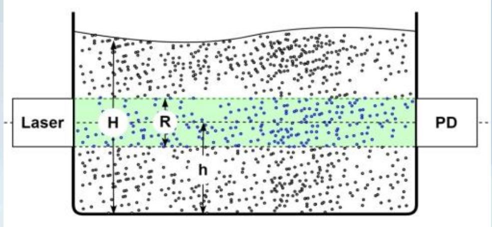
Introduction

One of the approaches to controlling the mechanical properties of dispersed-reinforced polymer composites is based on the formation of a polymer shell on the surfaces of dispersed particles of their filler. When formalizing mathematical models of the mechanical properties of such composites, the mechanical properties of the polymer matrix, dispersed particles, and also the polymer shell on the surfaces of these particles are taken into account. At the same time, the question of determining quantitative and numerical estimates of the mechanical properties of polymer shells remains open. It is not possible to directly measure the mechanical properties (Young's modulus, Poisson's ratio, and a number of others) of polymer shells. However, it is possible to determine the mechanical characteristics of polymer particles by assessing the molecular weight of the polymer and refining the required mechanical characteristics using known data. One of the approaches to measuring the molecular weight of a polymer is based on the analysis of the process and duration of sedimentation of polymer molecules and filler particles in a solvent. Based on the sedimentation time analysis, the weighted average molecular weight of the polymer is estimated.



The measuring system consists of a quartz container (Figure), into which a solvent, ethyl acetate, is poured. Particles of aluminum oxide (Al_2O_3) coated with polymer fibers are placed in the solvent and shaken. Under the influence of a solvent, the particles of aluminum oxide and polymer are separated. Under the influence of gravity and at a constant temperature, the particles begin to settle to the bottom of the quartz cell. Particle concentration measurements are based on Rayleigh scattering. Laser radiation is shone at the end of the quartz container, and a photodetector is installed at the other end. The output current of the photodetector is inversely proportional to the particle concentration. Over time, the particles will settle, and the total light transmitted through the container will also change. Based on the change in this luminous flux, it is possible to draw a conclusion about the current concentration of particles in the liquid. The task is to simulate the change in the optical power of the light flux passing through the quartz cell during the deposition of particles.

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Mathematical Model

$$M_i \frac{dW_i}{dT} = G_i - A_i - R_i$$

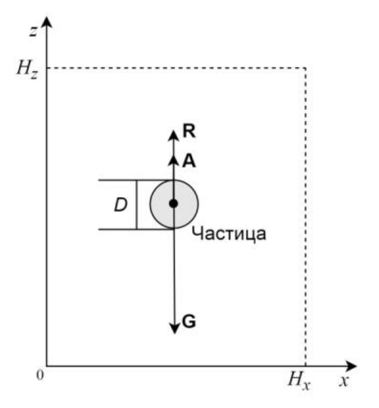
where:

$$A_i = -V_i \rho g = -\frac{\pi}{6} D_i^3 \rho g$$

$$R_i = -\xi(\mathrm{Re}) \frac{\rho W_i^2}{2} S_i$$

$$G_i = M_i g$$

$$\xi(\mathrm{Re}) = \frac{24}{\mathrm{Re}} \quad \mathrm{Re} = \frac{W_i D_i \rho}{\mu} \quad S_i = \pi \frac{D_i^2}{4}$$



The following variables are used in equations:

A_i – Archimedes force, G_i – gravity force, R_i – hydrostatic lifting force, W_i – velocity, M_i – mass of a particle, T – time, V_i – particles volume, D_i – particles diameter, ρ – liquids density, $\xi(\mathrm{Re})$ – dimensionless coefficient, S_i – cross-sectional area, Re – the Reynolds number, μ – fluid dynamic viscosity coefficient

Affection of Brownian motion of liquid

$$K_i = K_{\mathrm{T}} + \frac{(K_{\mathrm{B}} - K_{\mathrm{T}})}{H} z_i \qquad w_i^{\mathrm{B}} = \frac{w_i(m_i - m) + 2mw}{m_i + m}$$

$$E = \frac{mw^2}{2} \qquad N_{\mathrm{A}} = \frac{3}{2}\frac{RK}{E} \qquad m = \frac{M_{\mathrm{O}}}{N_A}$$

$$w_i^{\mathrm{BW}} = \frac{(N_{\mathrm{A}} m_i - M_{\mathrm{O}}) w_i + 2\sqrt{3\Re K_i M_{\mathrm{O}}}}{N_{\mathrm{A}} m_i + M_{\mathrm{O}}}$$

$$w_i^{\mathrm{B}} = \frac{(N_{\mathrm{A}} m_i - M_{\mathrm{O}}) w_i + 2\sqrt{3\Re K_i M_{\mathrm{O}}} \cdot \left(\mathrm{rnd}(1) - \frac{1}{2}\right)}{N_{\mathrm{A}} m_i + M_{\mathrm{O}}}$$

The following variables are used in equations:

K_{T} – the top liquid surface temperature, K_{B} – the bottom liquid surface temperature. K – temperature, E – kinetic energy of liquid's molecules, N_{A} – Avogadro's number, $\Re$ – universal gas constant, Mo – molar mass of liquid, w_i – particle velocity before exposure

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Particles Collisions

$$(w_i + w_j)\cdot\Delta t \le d_i + d_j \qquad w_i^{BH} = \sqrt{\left(w_i^{BW}\right)^2 - \left(w_i^{B}\right)^2}$$

$$\hat{m}_i = m_i + m_j \quad \hat{d}_i = \sqrt[3]{d_i^3 + d_j^3} \quad \hat{w}_i = \frac{m_i w_i + m_j w_j}{m_i + m_j} \quad \hat{z}_i = \frac{z_i + z_j}{2}$$

The following variables are used in equations:

z_i and z_j are coordinates, w_i and w_j are velocities S_H – area of horizontal surface of the container, w_i^{BH} – particle velocity in horizontal plane

The total luminous flux trapped by the particles

$$S(t) = \chi \sum_{i=1}^{N_1+N_2} \frac{\pi d_i^2}{4} \sqrt{1 - \left(\frac{z_i - h}{R}\right)^2} \qquad \text{where } h - R < z_i < h + R$$

The following variables are used in equation:

d_i – diameter, z_i – coordinate of a particle, χ – aspect ratio, H – height of the quartz container, R – radius of laser ray, h – laser ray height

The Equations in Dimensionless Form

$$M_i \frac{dW_i}{dT} = M_i g - \frac{\pi}{6} D_i^3 \rho g - 3\mu\pi D_i W_i$$

$$W_i = \frac{L_0}{T_0} \times w_i, \quad D_i = L_0 \times d_i, \quad M_i = M_0 \times m_i, \quad T = T_0 \times \tau$$

$$G_i = \left(\frac{T_0^2}{L_0} - \frac{\pi}{6} \frac{L_0^2 T_0^2}{M_0} \frac{d_i^3}{m_i} \rho\right) g, \quad R_i = -3\pi\mu \frac{L_0 T_0}{M_0} \frac{d_i}{m_i}$$

The Final Equations in Dimensionless Form

$$\boxed{\frac{dw_i}{d\tau} = G_i + R_i w_i}$$

The following variables are used in equations:

Characteristic values: L_0 – size, M_0 – mass, T_0 – time, K_0 – temperature. Dimensionless variables: w – speed, m – mass, d – diameter, τ – time.

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Initial Conditions

$$f(f_a, f_d) = f_a + f_d \cdot \sqrt{-2 \cdot \ln(\mathrm{rnd}(1))} \cdot \cos(2\pi \cdot \mathrm{rnd}(1))$$

$$d_i = \begin{cases} f(d_{T1}, \sigma_{dT1}), \\ f(d_{T2}, \sigma_{dT2}), \end{cases} \qquad \rho_i = \begin{cases} f(\rho_{T1}, \sigma_{\rho T1}), & 1 \le i \le N_1 \\ f(\rho_{T2}, \sigma_{\rho T2}), & N_1 < i \le N_1 + N_2 \end{cases}$$

The following variables are used in equation:

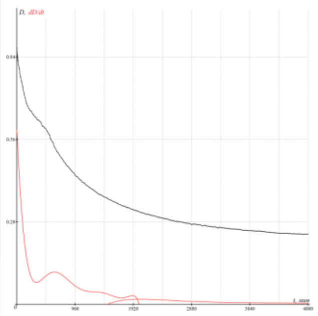
f_{avg} – mean, f_{disp} – dispersion, and rnd(1) – random values generator in the range [0, 1]. All particles are distributed in the liquid at the initial moment uniformly and with zero velocities, d_{T1} and d_{T2} – average diameters, σ_{dT1} and σ_{dT2} – size dispersions, ρ_{dT1} and ρ_{dT2} – average densities of particles, $\sigma_{\rho T1}$ and $\sigma_{\rho T2}$ – densities dispersions

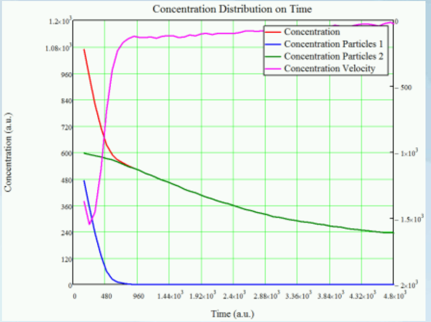
Finite Difference Scheme and Calculation Algorithm

$$\frac{w_i^{n+1} - w_i^n}{\Delta\tau} = (1-\theta)\left(G_i + R_i w_i^n\right) + \theta\left(G_i + R_i w_i^{n+1}\right)$$

$$w_i^{n+1} = \frac{(1 + (1-\theta)\Delta\tau R_i) w_i^n + \Delta\tau G_i}{(1 - \theta\Delta\tau R_i)}$$

Calculation Results





A numerical calculation was carried out for the deposition of particles of two types – aluminum oxide and polymer particles in ethyl acetate. The density of ethyl acetate ρ_{T1} = 902 kg/m^3, its viscosity μ = 0.40016×10^{-3} Pa·s. The density of particles of the first type (heavy, aluminum oxide Al_2O_3) ρ_{T1} = 7987 kg/m^3. The density of particles of the second type (light, polymer) ρ_{T1} = 3000 kg/m^3. The basic size of particles of the first type is d_{T1} = 0.25×10^{-6} m, of the second type d_{T1} = 0.125×10^{-6} m. The number of particles of the first type was taken equal to 1000, and of the second type, 10000.

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Conclusions

The result of the construction of mathematical models proposed in the work was the construction of a mathematical model for describing the deposition of two types of particles in a liquid. A complete two-dimensional mathematical model for describing the deposition of particles in a liquid at rest is proposed. The mathematical model takes into account the normal (Gaussian) distribution of particle sizes and densities. The equations of motion of particles under the action of gravity forces, hydrostatic buoyancy force of Archimedes, force of resistance to motion in a viscous fluid at low Reynolds numbers are written. It is proposed to write the equations of motion in a dimensionless form that is convenient for their numerical integration. The effect of Brownian (thermal) motion of liquid molecules on the velocity and movement of the deposited particles is taken into account on the basis of the elastic collision model. The speed of Brownian (thermal) motion of liquid molecules is related to the temperature of the liquid. The inelastic collisions of particles with each other are taken into account, in which the particles completely stick together, forming a new particle, with a new mass and velocity. Rayleigh scattering is modeled, which occurs when a laser beam passes through a quartz cell containing a solution with deposited particles. A computational algorithm for calculating the Rayleigh scattering value as a function of particle deposition over time is proposed.

A method is proposed for numerical simulation of measuring the concentration of particles of two types in a liquid based on Rayleigh scattering during their deposition. The mathematical model takes into account the forces of gravity, hydrostatic lifting force, forces of resistance to motion. Additionally, the contribution of the influence of Brownian fluid motion on the movement of suspended particles was taken into account. The magnitude of the scattering of the light flux as it passes through the volume of liquid with particles suspended in it is modeled. A numerical calculation was carried out according to the developed mathematical model.

Контакты

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