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## MATHEMATICAL MODELLING OF PARTICLE SETTLING AND CONCENTRATION STRATIFICATION IN A TWO-PHASE DISPERSED MIXTURE FLOW

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**Abstract.** This work develops a complete three-dimensional mathematical model for the gravitational settling of a two-phase dispersed mixture and the vertical stratification of concentration in a water reservoir, formulated within the framework of Kh.A. Rakhmatulin's theory of interpenetrating and interacting multiphase media. The system of mass and momentum conservation equations is written in Reynolds-averaged form and supplemented with the Boussinesq closure for turbulent diffusion and effective viscosity, together with the Stokes-Richardson-Zaki hindered settling law. The closure of the system is demonstrated by matching the eight unknown scalar functions with eight governing equations; physically grounded conditions are imposed on all six faces of the computational domain as well as at the initial time. Numerical computations carried out using a four-stage algorithm based on operator splitting and a finite-difference scheme on a staggered grid reproduce both qualitatively and quantitatively the time evolution of the concentration field, the formation of the clear-water/turbid interface, and the accumulation of the sediment layer.

**Keywords:** two-phase dispersed mixture, gravitational settling, stratification, Rakhmatulin model, hindered settling, turbulent diffusion, water reservoir.

### 1 INTRODUCTION

The clarification of water in reservoirs is a classical problem in hydraulic engineering and environmental hydrodynamics that, despite its long history, has not lost its relevance to the present day. The rivers of Central Asia – the Amu Darya, the Syr Darya, and the Zarafshan – are among the most sediment-laden waterways on Earth: the elevated concentration of suspended particles in their waters causes the rate at which regional reservoirs fill with sediment to substantially exceed the global average. The useful storage capacity of major reservoirs in Uzbekistan is shrinking year by year owing to sediment accumulation [13, 14]; for this reason, a reliable mathematical description of the stratification of a two-phase mixture inside such reservoirs is regarded as a primary task in the design of irrigation, industrial, and municipal water-supply systems.

The modern mathematical foundation for multiphase dispersed flows is provided by Kh.A. Rakhmatulin's concept of interpenetrating and interacting media [1]. In this approach each phase is characterised by its own velocity field and reduced density, while still being permitted to occupy the same spatial point simultaneously, and the interphase coupling is introduced through a dedicated interaction-force term. This framework presently underlies Euler–Euler type multiphase computational fluid dynamics models and has been successfully applied in industrial reactors and geophysical contexts [2].

The dependence of the settling dynamics on concentration – the transition from Stokes's formula to the hindered settling regime – has a long research history. The classical correlation of Richardson and Zaki [3] expresses the settling velocity as a power of the void fraction; the exponent depends on the particle Reynolds number and, at low values, lies close to four and a half. An extended analysis by Brzinski and Durian [4], based on twenty-seven experimental series, revealed that this exponent splits into two branches as a function of the Péclet number: about 5.6 in the Brownian regime and about 4.48 in the non-Brownian regime. For polydisperse systems, extended models have been proposed by Batchelor [5], Vowinckel et al. [6], and Chen et al. [7]; more recently, Ariff et al. [8] have compared the classical correlations against Stokesian simulations for log-normally distributed particles.

The mathematical theory of purely gravitational settling was founded by G.J. Kynch [9], who obtained a hyperbolic equation in the form of a nonlinear scalar conservation law for the concentration; the approach was subsequently extended by Bürger and co-workers [10] to a piecewise hyperbolic–parabolic framework,

giving rise to a shock-wave theory used in the design of industrial clarifier–thickeners and wastewater treatment units. The properties of turbulent diffusion and mixing in stratified turbulent flows have been investigated through the classical Miles-Howard theorem [11] and its successors; the most recent works [12] confirm the self-organisation of the gradient Richardson number around the critical value of one quarter on the basis of both field and laboratory measurements. Recent modelling efforts addressing sediment dynamics in reservoirs and lake-type water bodies [15] employ three-dimensional Reynolds-averaged systems; however, the majority of these treat the mixture as a single phase, using a single advection–diffusion equation with an effective density. In the present work we adopt the opposite stance, returning to a fully two-velocity formulation within the Rakhmatulin framework, since phase separation and the confusor effect can be represented directly only in such a scheme.

## 2 PROBLEM STATEMENT

A rectangular prismatic water reservoir with horizontal dimensions  $L_x \times L_y$  and depth  $H$  is considered. In a Cartesian coordinate system the  $x$  and  $y$  axes lie in the horizontal plane, the  $z$  axis points vertically upwards, and the origin is placed at the lower corner of the reservoir bottom. The computational domain is defined as:

$$\Omega = \{(x, y, z) : 0 \leq x \leq L_x, 0 \leq y \leq L_y, 0 \leq z \leq H\}. \quad (1)$$

The water in the reservoir is a two-phase dispersed mixture. The first phase is the carrier fluid – water of density  $\rho_f$  and dynamic viscosity  $\mu_f$ . The second phase consists of uniform spherical solid particles of diameter  $d$  and density  $\rho_s$ , with  $\rho_s > \rho_f$ . The particles are suspended in the water and settle downwards under gravity, while the water rises to fill the volume vacated by the particles. The side walls and the bottom of the reservoir are rigid and impermeable, whereas the upper surface, in contact with the atmosphere, is treated as a free surface. Inter-particle collisions, chemical reactions, thermal effects, and phase changes are neglected; among external forces only gravity is taken into account. Since the flow in real reservoirs is turbulent, the governing equations are written in the Reynolds-averaged sense, and from this point onwards all quantities denote time-averaged values; the influence of turbulent fluctuations is accounted for through effective-viscosity and turbulent-diffusion coefficients.

The principal unknown functions are: the volume fraction of particles  $\phi(\mathbf{r}, t) \in [0, 1]$ ; the water-phase velocity  $\mathbf{v}_1 = (u_1, v_1, w_1)$ ; the particle-phase velocity  $\mathbf{v}_2 = (u_2, v_2, w_2)$ ; and the pressure  $p(\mathbf{r}, t)$  – eight unknown scalar functions in total, where  $\mathbf{r} = (x, y, z)$ .

In the two-velocity Rakhmatulin scheme the mass and momentum conservation laws are written independently for each phase, while the coupling between phases is provided by the interaction force and a common pressure field. The Reynolds-averaged continuity equation for the particle phase, with the turbulent concentration flux modelled by a gradient-diffusion closure, takes the form:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{v}_2) = \nabla \cdot (D_t \nabla \phi), \quad (2)$$

where  $D_t$  is the turbulent diffusion coefficient. This equation combines, within a single balance, the local rate of change of concentration, the convective transport of particles by their own velocity, and the random diffusive spreading caused by turbulent fluctuations. For the water phase, which has concentration  $1 - \phi$ , the analogous equation reads:

$$-\frac{\partial \phi}{\partial t} + \nabla \cdot [(1 - \phi) \mathbf{v}_1] = -\nabla \cdot (D_t \nabla \phi). \quad (3)$$

The minus sign on the right-hand side is physically required: when particles diffuse away from a given region, water must enter to fill it, so that the diffusive fluxes of the two phases are oppositely directed. That this is consistent can be checked by summing (2) and (3): the diffusion terms cancel and one obtains the incompressibility condition for the volume-averaged mixture velocity,

$$\nabla \cdot \mathbf{V} = 0, \quad \mathbf{V} = (1 - \phi) \mathbf{v}_1 + \phi \mathbf{v}_2. \quad (4)$$

The physical meaning of (4) is that, because both phases of the mixture are incompressible, their combined volumetric flow is divergence-free: no volume is created or lost at any point.

The Reynolds-averaged momentum conservation equation for the particle phase, with turbulent stresses closed à la Boussinesq through the effective viscosity  $\mu_{\text{eff}} = \mu_f + \mu_t$ , can be written in the following vector form:

$$\phi \rho_s \left[ \frac{\partial \mathbf{v}_2}{\partial t} + (\mathbf{v}_2 \cdot \nabla) \mathbf{v}_2 \right] = -\phi \nabla p + \phi \mu_{\text{eff}} \nabla^2 \mathbf{v}_2 - \phi \rho_s \mathbf{g} + \beta(\phi) (\mathbf{v}_1 - \mathbf{v}_2), \quad (5)$$

where  $\mathbf{g} = (0, 0, g)$  is the gravitational acceleration vector and  $\mu_t$  is the turbulent viscosity. The factor  $\phi \rho_s$  on the left-hand side is the reduced density of the particle phase – the mass of particles per unit mixture volume – and the expression in brackets is the material derivative, i.e. the rate of change of velocity along a particle's trajectory. On the right-hand side, the first term represents the share of the pressure gradient acting on the particle phase: the factor  $\phi$  embodies the confuser effect characteristic of the Rakhmatulin model, namely the distribution of the pressure gradient over each phase in proportion to its volume fraction. The second term is the effective-viscosity force and combines the contributions of viscous stresses within the particle phase and turbulent Reynolds stresses; the third term,  $-\phi \rho_s \mathbf{g}$ , is gravity acting on the particle phase and constitutes the driving force of the settling process; the fourth term,  $\beta(\phi)(\mathbf{v}_1 - \mathbf{v}_2)$ , is the interphase drag exerted by the water on the particles and is proportional to the velocity difference between the two phases.

The momentum equation for the water phase is structurally identical, but with reduced density  $(1-\phi)\rho_f$  and with the sign of the interphase force reversed in accordance with Newton's third law:

$$(1-\phi)\rho_f \left[ \frac{\partial \mathbf{v}_1}{\partial t} + (\mathbf{v}_1 \cdot \nabla) \mathbf{v}_1 \right] = -(1-\phi)\nabla p + (1-\phi)\mu_{\text{eff}} \nabla^2 \mathbf{v}_1 - (1-\phi)\rho_f \mathbf{g} - \beta(\phi) (\mathbf{v}_1 - \mathbf{v}_2). \quad (6)$$

Projecting (5) and (6) onto the three coordinate directions yields three momentum equations each, for a total of six scalar momentum equations.

The interphase interaction coefficient, obtained by generalising the Stokes drag law for a single spherical particle to a many-particle system, is given by:

$$\beta(\phi) = \frac{18 \mu_f \phi}{d^2} (1-\phi)^{1-n_R}, \quad (7)$$

where  $n_R$  is the hindrance exponent introduced by Richardson and Zaki [3]. Let us examine the mechanics of the settling process in more detail. A single spherical particle moving in the fluid is subject to three forces: gravity  $F_g = (\pi d^3 / 6) \rho_s g$ , the Archimedes buoyancy force  $F_A = (\pi d^3 / 6) \rho_f g$ , and the Stokes drag force  $F_d = 3\pi \mu_f d w$ . In the steady regime, the force balance  $F_g - F_A - F_d = 0$  yields the Stokes settling velocity of a single particle,

$$w_{\text{St}} = \frac{(\rho_s - \rho_f) g d^2}{18 \mu_f}. \quad (8)$$

This formula is valid when the particle Reynolds number  $\text{Re}_p = \rho_f w_{\text{St}} d / \mu_f < 1$  – that is, in the slow-settling regime of small particles. In real reservoirs the particles do not settle in isolation; rather, a large number of particles settle simultaneously, and as the concentration rises, hydrodynamic interactions between particles and the return flow of displaced fluid both reduce the settling velocity substantially. This combined effect, known as hindered settling, leads – once the interphase coefficient is inserted into the momentum equations – to an effective settling velocity of the form:

$$w_s(\phi) = w_{\text{St}} (1-\phi)^{n_R}. \quad (9)$$

Relation (9) has important limiting cases:  $\phi \rightarrow 0$  gives  $w_s \rightarrow w_{\text{St}}$ , recovering the maximum settling velocity in the single-particle regime;  $\phi \rightarrow 1$  gives  $w_s \rightarrow 0$ , so that motion ceases in a densely packed assembly. For low  $\text{Re}_p$ , the experiments of Richardson and Zaki [3] established  $n_R \approx 4.65$ ; however, according to the analysis of Brzinski and Durian [4], as the Péclet number of the particles crosses the boundary between the Brownian and non-Brownian regimes, the exponent varies from about  $n_R \approx 5.6$  to

about  $n_R \approx 4.48$ . For the typical turbid particles found in water reservoirs, the non-Brownian branch is the relevant one for practical purposes. The system therefore constitutes a complete mathematical model of the settling and stratification process in a two-phase dispersed mixture: eight unknown functions  $\mathbf{v}_1$ ,  $\mathbf{v}_2$ ,  $p$ ,  $\phi$  – and eight equations (two continuity and six momentum equations), so that the system is closed.

For the problem to be physically well-posed, all unknown functions must be specified at  $t=0$  throughout  $\Omega$ :

$$\phi(\mathbf{r}, 0) = \phi_0(\mathbf{r}), \mathbf{v}_n(\mathbf{r}, 0) = \mathbf{v}_{n0}(\mathbf{r}) \quad (n=1,2), p(\mathbf{r}, 0) = p_0(\mathbf{r}). \quad (10)$$

The function  $\phi_0$  describes the initial turbidity of the reservoir, while  $\mathbf{v}_{n0}$  encodes any initial flow field generated by incoming streams, wind action, or other external forcing. The most common situation in practice is that the reservoir is at rest and the particles are uniformly distributed; in this case:

$$\phi_0 = \text{const}, \mathbf{v}_{n0} = 0, p_0(z) = p_{\text{atm}} + [\rho_f(1-\phi_0) + \rho_s\phi_0] g(H-z), \quad (11)$$

and the resulting expression for the pressure corresponds to a hydrostatic distribution.

The boundary  $\partial\Omega$  of the computational domain comprises six faces, on each of which physically grounded conditions are imposed. The bottom of the reservoir is a rigid, impermeable, horizontal surface; for the water phase the no-slip condition is enforced, while for the particle phase the horizontal velocities vanish and the vertical velocity equals the settling velocity – particles continue to settle once they reach the bottom:

$$\mathbf{v}_1|_{z=0} = 0, u_2|_{z=0} = v_2|_{z=0} = 0, w_2|_{z=0} = -w_s(\phi|_{z=0}). \quad (12)$$

The boundary condition for the concentration on the bottom expresses the balance between the convective and diffusive fluxes,

$$(-\phi w_s + D_t \partial_z \phi)|_{z=0} = q_b(x, y, t), \quad (13)$$

where  $q_b$  is the rate of sediment accumulation on the bottom. If the bed fully absorbs the sediment, then  $q_b = \phi w_s|_{z=0}$  and the diffusive flux vanishes.

The upper face of the reservoir is in contact with the atmosphere and is treated as a free surface. In the absence of wind, the tangential stresses vanish, the kinematic condition for the vertical velocity expresses the impermeability of the free surface, and the pressure equals the atmospheric value:

$$\partial_z u_1|_{z=H} = \partial_z v_1|_{z=H} = 0, w_1|_{z=H} = 0, p|_{z=H} = p_{\text{atm}}. \quad (14)$$

Particles do not escape through the free surface, so that the total flux – the sum of gravitational settling and turbulent diffusion – vanishes there:

$$(-\phi w_s + D_t \partial_z \phi)|_{z=H} = 0. \quad (15)$$

At the side walls  $x=0, L_x$  and  $y=0, L_y$  impermeability conditions are imposed,

$$u_n|_{x=0, L_x} = 0, v_n|_{y=0, L_y} = 0 \quad (n=1,2), \partial_n \phi|_{\partial\Omega_{\text{side}}} = 0, \quad (16)$$

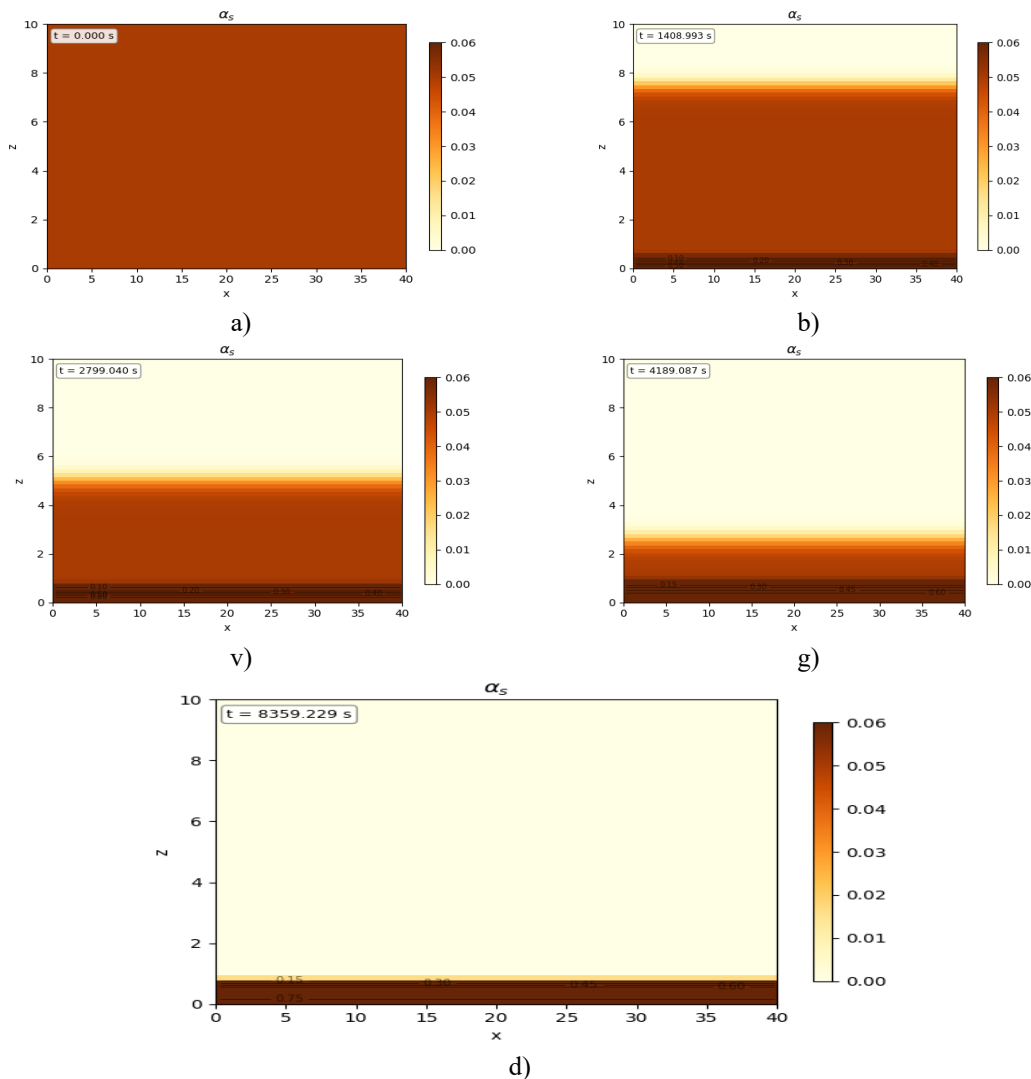
the last of which expresses the vanishing of the diffusive flux of particles through the walls.

### 3 RESULTS AND DISCUSSION

To solve the formulated problem, a four-stage numerical algorithm based on a finite-difference operator-splitting scheme for the coupled system of eight unknowns has been developed. The algorithm relies on a Harlow–Welch-type staggered grid, which prevents spurious oscillations between pressure and velocity. The advective terms are discretised conservatively to second order using a TVD reconstruction with the minmod limiter, while the diffusive and viscous terms are treated implicitly via a Crank–Nicolson scheme combined with an ADI strategy, so that stability is constrained only by the advective CFL condition. The interphase interaction term is handled semi-implicitly, eliminating the singularity at high concentrations; together with gravity, it is accounted for directly through the analytic solution of the corresponding two-equation coupled phase subsystem. The incompressibility constraint is enforced through a pressure-correction step and a Poisson equation, which is solved efficiently by a preconditioned conjugate-gradient (PCG) method with an incomplete Cholesky preconditioner, while the nonlinear

coefficients are updated by Picard iteration. The reliability of the algorithm has been verified against Kynch's analytical solution [9], the characteristic clarification time, mass conservation, grid convergence, and an estimate of the operator-splitting error.

The computational domain and the physical parameters were chosen so as to model a typical sedimentation pond – for example, the settling basin of a local reservoir. The horizontal dimensions were taken as  $L_x = 40 \sim \text{m}$  and  $L_y = 20 \sim \text{m}$  and the depth as  $H = 10 \sim \text{m}$ , corresponding to a moderately wide and moderately deep reservoir configuration. The particle diameter is  $d = 5 \cdot 10^{-5} \sim \text{m}$  ( $50 \sim \mu\text{m}$ ) – consistent with fine quartz sand or a coarse clay fraction – and the particle density is  $\rho_s = 2650 \sim \text{kg/m}^3$ . The initial concentration  $\phi_0 = 0.05$  is a representative average value for a typical turbid inflow. The grid resolution was set to  $N_x = 80$ ,  $N_y = 40$ ,  $N_z = 64$ , giving horizontal spacings  $\Delta x = \Delta y = 0.5 \sim \text{m}$  and a vertical spacing  $\Delta z = 0.15625 \sim \text{m}$ . The vertical refinement ( $\Delta z \approx \Delta x / 3$ ) is intended to resolve adequately the sharp concentration gradients associated with the settling velocity – in particular, the clear-water/turbid interface.



**Fig. 1.** Time evolution of the concentration field in the midplane  $y = L_y / 2$  at five characteristic instants: (a)  $t = 0$ ; (b)  $t \approx T_{cl} / 4$ ; (c)  $t \approx T_{cl} / 2$ ; (d)  $t = T_{cl}$ ; (e)  $t \approx 1.5 T_{cl}$

The results presented in Figure 1 reveal the following patterns. At the initial instant ( $t = 0$ ),  $\phi(x, z)$  retains its uniform value of 0.05 throughout the domain and appears as a single yellow-brown colour in the visualisation. As time progresses, two distinct stratification processes develop simultaneously: the formation of a clear-water zone propagating from the top downwards, and the accumulation of a sediment layer building up from the bottom. At  $t \approx T_{cl} / 4 = 1408 \sim \text{s}$ , in the region  $z > 8 \sim \text{m}$  near the free surface the concentration drops from 0.05 to values below 0.01 – a clarified layer has formed – while in the region

$z < 0.5 \sim m$  near the bottom the concentration starts to increase steadily. At the next instant ( $t = 2799 \sim s$ ), the clear-water/turbid interface has reached a depth of  $z \approx 5 \sim m$ , and the  $\phi = 0.025$  isoline (half of the initial value) marks its precise location. At  $t = 4189 \sim s$  the clear zone has expanded further, with the interface descending to  $z \approx 2.5 \sim m$ . At the time  $t = T_{cl} = 5646 \sim s$  predicted by Kynch theory, the clear-water front practically reaches the upper boundary of the sediment layer; from this moment onwards, the simulation shows a sharp slowdown in the descent of the interface – the practical manifestation of the nonlinear braking effect. Finally, at  $t = 8359 \sim s$  ( $\approx 1.5 T_{cl}$ ), the domain is divided into two clearly defined zones: a dense sediment layer of height approximately  $0.86 \sim m$  and the remaining  $9.14 \sim m$  of essentially clear water above. These results confirm, on the one hand, the quantitative agreement of the model with the predictions of Kynch–Bürger hyperbolic theory [9, 10] and, on the other hand, the leading role played by phase separation and the confusor effect – features intrinsic to the Rakhmatulin model – in shaping the stratified structure.

## 4 CONCLUSION

In the present work, a complete three-dimensional mathematical model (2)–(9) for the settling of dispersed particles and the stratification of concentration in a water reservoir has been developed within the Rakhmatulin theory of two-phase media, and its initial (10)–(11) and boundary (12)–(16) conditions have been justified on physical grounds. The system consists of eight unknown functions and eight equations and is therefore mathematically closed. The particle settling velocity is expressed through a Stokes–Richardson–Zaki hindered-settling law (9), whose internal coupling with the interphase coefficient (7) and the momentum equations (5)–(6) has been made explicit. Numerical computations performed with the finite-difference operator-splitting algorithm on a staggered grid faithfully reproduce, both qualitatively and quantitatively, the time evolution of the concentration field, the formation of the clear-water/turbid interface, the nonlinear braking near the Kynch characteristic time  $T_{cl}$ , and the final height of the sediment layer.

The model offered here has two important features. First, the confusor effect of Rakhmatulin’s scheme allows the interphase interaction to be represented directly: unlike a single-velocity Boussinesq-type approximation, it makes possible the explicit modelling of phase separation dynamics. Second, the model is fully consistent with the classical Kynch–Bürger hyperbolic theory [9, 10] and thus preserves continuity with the modern frameworks currently employed in industrial clarifier–thickeners and wastewater treatment units. The results obtained provide a theoretical basis for further numerical modelling and for the applied design of water reservoirs.

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## МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ОСАЖДЕНИЯ ЧАСТИЦ И СТРАТИФИКАЦИИ КОНЦЕНТРАЦИИ В ДВУХФАЗНОМ ПОТОКЕ ДИСПЕРСНОЙ СМЕСИ

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**Аннотация.** В данной работе разработана полная трехмерная математическая модель гравитационного осаждения двухфазной дисперсной смеси и вертикальной стратификации концентрации в водохранилище, сформулированная в рамках теории взаимопроникающих и взаимодействующих многофазных сред Х.А. Рахматулина. Система уравнений сохранения массы и импульса записана в форме, усредненной по Рейнольдсу, и дополнена замыканием Буссинеска для турбулентной диффузии и эффективной вязкости, а также законом замедленного осаждения Стокса-Ричардсона-Заки. Замыкание системы демонстрируется путем сопоставления восьми неизвестных скалярных функций с восемью управляющими уравнениями; на всех шести гранях расчетной области, а также в начальный момент времени, накладываются физически обоснованные условия. Численные вычисления, выполненные с использованием четырехэтапного алгоритма, основанного на расщеплении операторов и конечно-разностной схеме на шахматной сетке, качественно и количественно воспроизводят временную эволюцию поля концентрации, формирование границы раздела чистая/мутная вода и накопление осадочного слоя.

**Ключевые слова:** двухфазная дисперсная смесь, гравитационное осаждение, стратификация, модель Рахматулина, затрудненное осаждение, турбулентная диффузия, водохранилище.