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New model of the sedimentation process of polydisperse post-coagulation suspension

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Abstract. Coagulation is a process during which a flocculent suspension may sediment. It is characterized by its polydisperse structure. There are three main fractions of sedimentation particles after coagulation: spherical, non-spherical and porous agglomerates. Each of the fractions sediments in a different manner, for different forces act on them, due to interactions between the particles, inhibition or entrainment of neighboring particles. The existing sedimentation models of polydisperse suspension do not consider the flocculation process, i.e. the change of one particle into another during sedimentation, resulting from their agglomeration. The presented model considers the shape of particles and flocculation, which is a new approach to the description of the mathematical process of sedimentation. The velocity of sedimentation depends on the concentration of particles of a given fraction in a specific time step. Following the time step, the heights of individual fractions are calculated. Subsequently, new concentration values of individual fractions are determined for the correspondingly reduced volume of occurrence of a given fraction in the volume analyzed, taking particle flocculation into consideration. The new concentration values obtained in this way allow to recalculate the total sedimentation rates for the next time step. Subsequent iterations allow for numerical simulation of the sedimentation process.

Key words: sedimentation modelling; polydisperse suspension; iterative model.

1. INTRODUCTION

Coagulation is widely used in the conditioning of potable and industrial water, in wastewater treatment and in the treatment of leachate from landfills. Coagulation is a chemical method used for water and wastewater treatment [1–4]. It is an important process for the conditioning of water in conventional water and wastewater treatment plants. During the process, colloidal particles causing turbidity and producing color are removed from the water, together with non-sedimentation suspensions and organic contaminants, including the precursors of by-products of chemical disinfection and oxidation, as well as many micro-contaminants. Colloidal solutions form molecules and ions with a diameter of 1–100 nm, forming a micro-homogeneous system referred to as a colloidal or dispersive system. The coagulation process involves the addition of coagulant to the purified suspension/water, which reduces the degree of dispersion of the colloidal system [5, 6]. The addition of coagulant causes small particles to form larger clusters – agglomerates – which are then removed from the water through sedimentation, flotation and filtration. Coagulation particles have different shapes, sizes and porous structures [7–9]. Depending on the type of the treated medium, flocs may be formed which sediment at different velocities, and their mass and shape change as they sediment. Such a suspension has a polydisperse structure, which is why a mathematical approach to the problem of sedimentation of these suspensions is not easy. Sedimentation is an extensively applied process, which has not been sufficiently described mathematically yet. This results from the complexity of this phenomenon, which consists, among others, of the interaction between particles and between particles and walls of the vessel, the shape, dimension, density and concentration of sedimentation particles, density, temperature, velocity and direction of flow [10–13]. This paper presents a numerical iterative model of the sedimentation of particles of a coagulation suspension for 3 groups of particles: spherical, non-spherical and porous agglomerates. Mutual interactions between particles and changes in concentration of particular groups of particles during their descent are assumed.

2. RESEARCH PROBLEM

During sedimentation, particles interact with each other, which disturbs their movement. For the mathematical description of this phenomenon, it is not possible to apply equations for the free fall of bodies. The most important parameter for the sedimentation process is the parameter of particle sedimentation velocity. Concentration of particles [14–17] has a large influence on sedimentation velocity. The process of sedimentation is very complex and most often, in order to determine the rate of sedimentation for a real suspension, it is necessary to conduct experimental studies. Figure 1 presents a polydisperse coagulation suspension. The diverse shape of individual particles influences the way they fall down. Spherical particles have a compact structure, so their sedimentation follows a straight track with a slight zigzag motion. The movement is sometimes dis-

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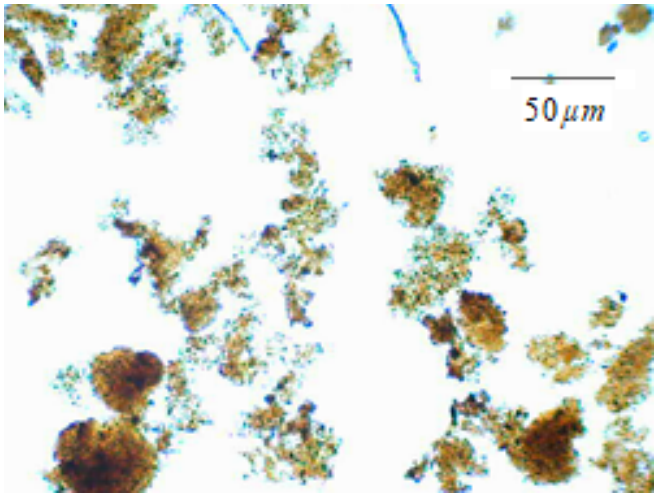

Fig. 1. Microscopic image of a polydisperse coagulation suspension

turbed by particles of larger dimensions, moving in their vicinity. Sedimentation of non-spherical particles involves a rotary motion around their own axis and moving along a spiral track. Spherical and non-spherical particles may merge into larger agglomerates over time. Agglomerates have macropores through which the liquid can flow during their movement, which resembles flowing through a porous deposit. For this type of particles, the rotary motion around their axis disappears and they fall in a straight-line motion.

3. SEDIMENTATION PROCESS MODELING

The process of polydisperse mixture sedimentation is relatively complicated. There are few models in the literature describing such processes [18, 19]. One way is to describe the polydisperse mixture with the use of models for monodisperse sedimentation, introducing average values of particles concentration and density [14, 15, 20]. Such an approach only applies to suspensions, in which the particles do not differ significantly from each other both in shape and density.

One of the most popular models is the Richardson and Zaki model [21]. They proposed to determine the velocity of sedimentation on the basis of known values of sedimentation velocity for a single particle. As the liquid near the particles starts to circulate when more particles are in motion, some of the liquid moves upwards as the particles move downwards. This causes the sedimentation velocity of a group of particles to decrease beyond the value of the free-fall velocity of a single solid particle. The Richardson and Zaki model was later modified by other researchers [22–26].

In their studies on polydisperse colloidal suspension, Biesheuvel [27] *et al*. considered that there was a layer of sediment and a clear supernatant. The Patwardhan and Tien [28] model for describing particle velocities in polydisperse systems applied closed continuous equations [27]. These equations can be derived from macroscopic momentum balances (Syamlal and O'Brien [29]) and show that the driving force of sedimentation is the difference in density of a given ρ particle with the entire density ρ_s of the suspension at this location. Expressions about particle velocity include empirical hindrance functions for polydisperse systems based on those obtained in 1954 by Richardson and Zaki for monodisperse systems.

When modeling the sedimentation of polydisperse suspensions, particle size distribution and density distribution should be taken into account. Accordingly, the number of parameters describing the sedimentation process is bound to increase. It is possible that, instead of falling, small particles of low density will be carried up along with the movement of the liquid, which is caused by the sedimentation of particles of larger dimensions and densities.

The method of calculating the sedimentation velocity for a suspension, consisting of two fractions of different dimensions and different densities, based on a cellular model, requires the introduction of the concept of effective concentration. Namely, the concentration of solids in a k_j cell of d_{ej} in diameter. This model assumes that the particle inside the cell moves at velocity v_j while the liquid in this cell has the velocity of v_{cj}. Smith [30] developed a formula for calculating the velocity difference between a moving particle and the surrounding liquid. The formula proposed by Smith was modified many times by other researchers [31, 32].

Richardson and Shabi observed that four zones are formed for spherical suspensions of two dimensions and equal density: a clean liquid zone, a smaller particle suspension zone, a larger particle suspension zone and a sediment zone. On this basis, they proposed a zone model [33, 34], in which the velocity of movement of borders between zones is considered. The idea of the model is presented in Fig. 2. The velocity of sedimentation of the particles in individual zones is calculated in the same manner as for a monodisperse suspension.

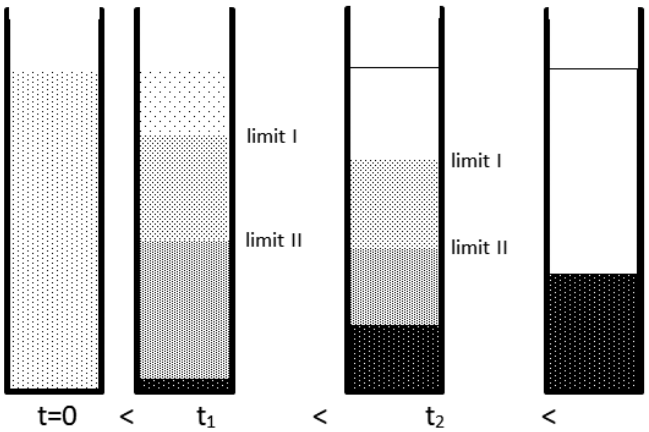

Fig. 2. Model course of the process of sedimentation of a polydisperse mixture; source: own study

The most difficult task is to model the sedimentation process for particles of different sizes and densities [35]. A model for such a process was presented by Zimmels [36]. The author ignores the influence of collisions of particles and assumes that the disturbance of the motion of particles depends on the total volumetric share. He further assumes that the distribution of

concentration of particles is uniform throughout the suspension. This model is presented both for a suspension of N of different fractions of the same density and for a suspension of N of different fractions, and m of different densities.

4. OWN SEDIMENTATION PROCESS MODEL OF THE COAGULATION SUSPENSION

The models of sedimentation of polydisperse mixtures described so far do not allow for the interaction of individual fractions. The sedimentation velocity of a selected fraction is strongly influenced by the concentration value of the remaining fractions. Therefore, a model was proposed that acknowledges the mutual influence of fraction concentration on sedimentation velocity. Furthermore, particles may have different densities, sizes and shapes.

The models of polydisperse suspension sedimentation present in available literature do not consider the interactions between molecules during their sedimentation. This paper presents a model which allows for both, the interactions between sedimentation molecules and the concentration of individual fractions. The concentration of fractions affects the velocity of sedimentation in a polydisperse suspension. The fractions differ in density, size and shape. The model was developed for a polydisperse suspension consisting of three fractions with different mechanisms of sedimentation.

In order to describe the behavior of polydisperse suspensions, it is required, unlike for monodisperse suspensions, to define additional variables characterizing the distribution of properties of solid particles. In practice, polydisperse suspensions are most often described by:

- the distribution of particle diameters and their uniform density;
- the same diameter of particles and the distribution of their density;
- a single particle diameter distribution and a single particle density distribution;
- multiple distributions of particle diameters and their densities.

4.1. Selecting a template

A model coagulation suspension consisting of three basic fractions was prepared. Figure 3 presents three basic groups of particles occurring in the prepared polydisperse mixture. Three groups of particles can be distinguished: spherical, non-spherical and porous agglomerates.

4.2. Numerical iterative model

The model assumes that the sedimentation process begins when there is a homogeneous mixture with a differentiated volumetric share of individual fractions (Fig. 4a) in the whole analyzed volume. The assumption is that in successive time steps t_n the amount by which the individual fractions fall is calculated. Heights h_{I}, h_{II} and h_{III} are calculated on the basis of sedimentation velocity. Assuming that the analyzed volume is constant, the volume fraction of individual fractions changes. The analyzed volume is limited by dashed lines. Sample process flow:

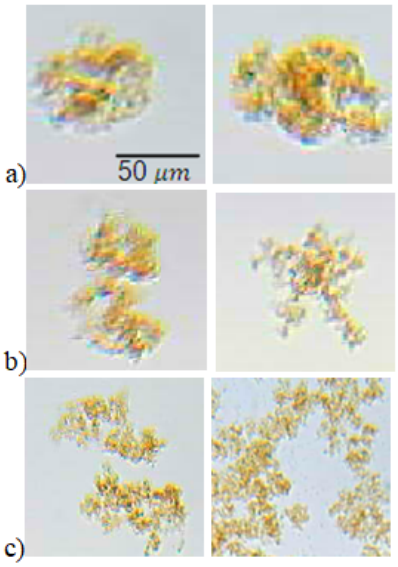

Fig. 3. Types of particles occurring in the process of sedimentation of a coagulation suspension a) spherical, b) non-spherical, c) porous agglomerates, own sources

at the beginning of the process, it is assumed that the analyzed volume contains a homogeneous mixture of all three fractions (Fig. 4a). After a certain time step, a clear liquid is formed from the liquid surface – height h_o to height h_{I}. Between h_{I} and h_{II} there is no longer fraction III and II, only fraction I, from height h_{II} to h_{III} there is no longer fraction III, only fraction II and I, from h_{III} down the vessel is still a homogeneous mixture of all three fractions. In subsequent time steps in the analyzed volume, the positions of heights h_{I}, h_{II} and h_{III} change (Fig. 4b, 4c). Changes in height make it possible to calculate the falling rates of individual fractions in an iterative way for successive time steps. The numerical iterative method then calculates the change of concentration of individual phases in the selected cross-sectional space of the sedimentary column for subsequent intervals. In the first phase, the sedimentation velocities of individual fractions are calculated. After the first interval, when there is a change in the volumetric share of individual fractions in the analyzed volume, the sedimentation velocities of the individual fractions are recalculated (Fig. 4b). This way, the subsequent intervals of the process are iteratively modeled.

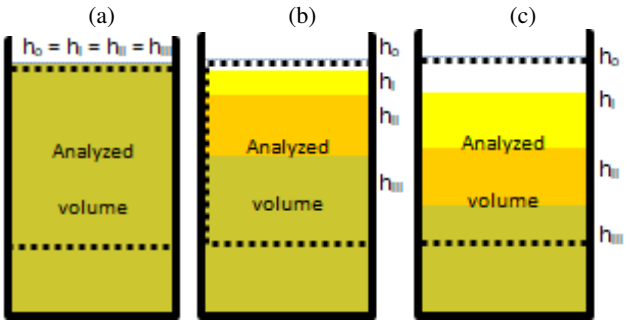

Fig. 4. Model of sedimentation of a polydisperse mixture: a) beginning of the sedimentation process, b) movement of individual fractions after t_1, c) movement of fractions after t_2. Source: own study

The presented model concerns the sedimentation process with simultaneous flocculation, it thus includes the modeling of two processes.

4.3. Sedimentation modeling

Modeling begins with the calculation of the sedimentation velocity of selected fractions for known values of mass concentrations of individual fractions Φ_{Io}, Φ_{Io} and Φ_{IIIo}. The sedimentation velocity of individual fractions is calculated as for a monodisperse mixture for v_{Is}, v_{IIs} and v_{IIIs} [37].

Cellular models are popular in literature [22–24]. They assume that cells are evenly distributed in liquids. Each of the cells consists of a fluid, inside which there are solid particles. This model considers the volume share of particulates in the fluid volume. The basic equation describing the relationship between the sedimentation velocities of individual fractions, including the movement of liquids and the velocity of sedimentation of individual fractions for a monodisperse mixture, is:

$$v_{Is} = v_{Iso}\frac{1}{1+n\Phi_{I0}^{1/3}}, \tag{1}$$

$$v_{IIs} = v_{IIso}\frac{1}{1+n\Phi_{II0}^{\frac{1}{3}}}, \tag{2}$$

$$v_{IIIs} = v_{IIIso}\frac{1}{1+n\Phi_{III0}^{1/3}}, \tag{3}$$

where: Φ – volumetric share (concentration) of particulate matter in the suspension; v_{Is0}, v_{IIs0}, v_{IIIs0} – sedimentation velocities of individual fractions, taking into account the movement of liquids, m/s.

A value of n equal to 1.5 was initially proposed by Happel and Epstein [24], but Barnea and Mizrahi [25] specified that this value should be in the range of 1–2.1, depending on the type of suspension.

Sediment particles cause the liquid in their vicinity to move. Movement of the liquid may cause the descent rate to change, which is important for small particles. This is the basis for correcting the sediment velocity of the selected fraction by the movement of the liquid caused by sedimentation of the entire suspension.

$$v_{Iso} = v_{Io} - v_c\,, \tag{4}$$

$$v_{IIso} = v_{IIo} - v_c\,, \tag{5}$$

$$v_{IIIso} = v_{IIIo} - v_c\,. \tag{6}$$

The velocity v_c of liquid movement caused by the sedimentation of various fractions of the suspension, should be calculated using the following formula:

$$v_c = \frac{1}{1-\Phi_z}\sum_{j=1}^{N} v_j\Phi_j\,, \tag{7}$$

where the total concentration equals:

$$\Phi_z = \sum_{j=1}^{N}\Phi_j\,. \tag{8}$$

Equations (4)–(6) provide the basis for calculating the sedimentation velocity of individual fractions of the polydisperse mixture. However, they only regard the interaction between particles. In practice, during their movement, numerous collisions of particles belonging to different fractions occur, which causes a change in their velocity of movement. The impact of collisions on the velocity of sedimentation of individual fractions can be generally described by equations for inelastic collisions.

Velocity v_{I0} stands for the free-fall of a single particle in a still liquid. Due to different mechanisms of sedimentation, depending on the individual groups separated from the coagulation suspension, v_{I0}, v_{II0}, v_{III0} velocities are calculated from the dependencies described below.

Spherical particles fall freely, and the velocity of the sedimentation analysis is based on Stokes' law, which is also referred to as the relation for sedimentation rate. It was derived in 1851 by George Gabriel Stokes [3, 15, 16]. The basic distribution of forces acting on a particle during its sedimentation is shown in Fig. 5.

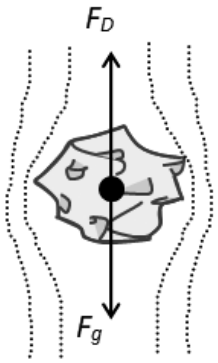

Fig. 5. Forces acting on a spherical particle. Source: own study

The velocity of the particle is influenced by two basic forces: the gravity force always facing downwards F_g and the drag force opposite to the direction of motion F_D. The force of gravity F_g was defined according to Archimedes' principle, taking the porosity of the material into account:

$$F_g = (\rho_s - \rho_l)\,gV_s(1-\varepsilon_I), \tag{9}$$

where: ρ_s – sediment density, kg/m^3; ρ_l – liquid density, kg/m^3; g – gravity acceleration, m/s^2; V_s – particle volume, m^3; ε_I – sediment porosity.

In the literature, F_D drag force is defined as the following formula [16, 17]:

$$F_D = C_D A_s \rho_l \frac{v_0|v_0|}{2}\,, \tag{10}$$

where: C_D – drag coefficient; A_s – cross-sectional area of the particle in the horizontal plane, m^2; v_o – particle sedimentation velocity, m/s.

The shape of particles has a direct influence on the rate of their sedimentation and the value of the coefficient of drag C_D [38, 38–42]. The determination of the drag coefficient de-

pends on the type of flow in the liquid, which is defined by the Reynolds number.

For small values of the Reynolds number, it is assumed that [43–45]:

$$\mathrm{Re} \leq 0.3, \quad C_D = \frac{24}{\mathrm{Re}}. \tag{11}$$

In the range of $\mathrm{Re} \leq 0.3$ the coefficient is taken as $C_D = \frac{24}{\mathrm{Re}}$. As per formulas (9), (10), (11), the final formula for velocity of sedimentation of a single particle will match the balance of forces acting on it in the process, and takes the following form:

$$v_{\mathrm{I}0} = \frac{(\rho_s - \rho_l)\, g d_{\mathrm{I}e}^2 (1 - \varepsilon_{\mathrm{I}})}{18 \eta_l}, \tag{12}$$

where: $d_{\mathrm{I}e}$ – equivalent particle diameter of fraction I, m; η_l – liquid viscosity, Pa · s.

Tests consisting in the sedimentation velocity of the suspension of microparticles were carried out, hence measuring the sedimentation velocity of the suspension consisted only of selected particles of fraction I, for which the sedimentation velocity of a single particle was determined, including the dependences (formulas (1) and (4)), for which the Φ concentration was determined by means of the microscopic method. The results of changes in sedimentation velocity depending on concentration are shown in Fig. 6:

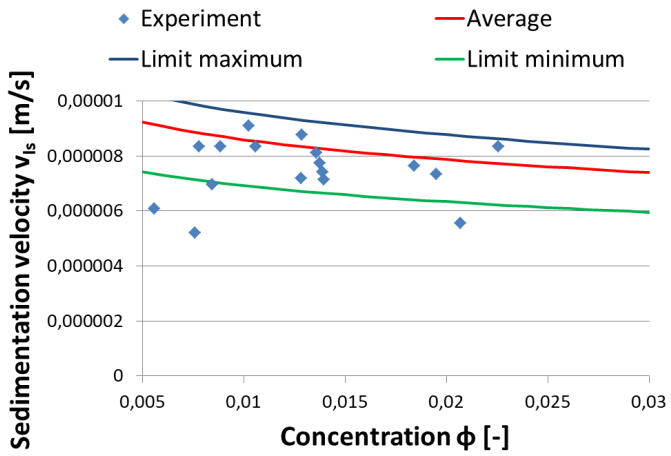

Fig. 6. Dependence of sedimentation velocity of monodisperse suspension of fraction I on the Φ concentration of this fraction, own study

The green and gray curves in the graph define the particle diameter limits for the minimum and maximum particle diameters and for the epsilon limit values. The red line in the center shows the result for the diameter and the epsilon resulting from the diameter distribution and epsilon distribution. This line constituted the basis for the verification of the C_D drag coefficient. The C_D coefficient was experimentally determined. After verification with experimental data, it turned out that the drag coefficient was selected correctly.

Non-spherical particles move along non-linear paths. This disturbs the movement of the liquid around the settling particle and results from a lateral force. The result is a lateral force perpendicular to the direction of motion F_M (Fig. 7). For low velocities of motion this force can be neglected in calculations, however, the irregular shape of the particles makes their motion curvilinear anyway. The reason is that the particle slips or flows down in the direction transverse to the axis of the column. Mathematical description of all phenomena that occur during such a movement is impossible in practice due to the large diversity of particle shapes.

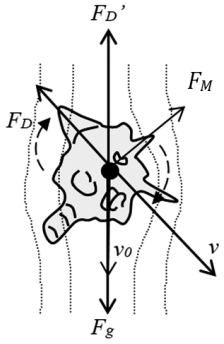

Fig. 7. Forces acting on a non-spherical particle. Source: own study

The vertical velocity of sedimentation of non-spherical particles is dependent on the balance of forces acting upon it. In this case, the greatest influence is exerted by the force of drag to sedimentation F_D', which is a resultant of the drag force of motion F_D and lateral force action F_M [46–49]. The drag of motion F_D is calculated using equation (10).

The resultant value of the drag force in the vertical direction can be calculated with the formula below:

$$F_D' = \sqrt{F_D^2 + F_M^2}. \tag{13}$$

The force of F_D and the force of F_M are two forces that can be expressed with relationship (13), differing in the value of the C_D coefficient. By denoting respectively the coefficients C_D for force F_D and C_M for force F_M, the equation for force F_D' takes the following form:

$$F_D' = \sqrt{\left(C_D \frac{\pi d_{\mathrm{II}e}^2}{4} \rho_l \frac{v_{\mathrm{II}o}^2}{2}\right)^2 + \left(C_M \frac{\pi d_{\mathrm{II}e}^2}{4} \rho_l \frac{v_{\mathrm{II}o}^2}{2}\right)^2}, \tag{14}$$

$$F_D' = \sqrt{\left(\frac{\pi d_{\mathrm{II}e}^2}{4} \rho_l \frac{v_{\mathrm{II}o}^2}{2}\right)^2 \left(C_D^2 + C_M^2\right)}, \tag{15}$$

where: $d_{\mathrm{II}e}$ – equivalent particle diameter of fraction II, m; $v_{\mathrm{II}o}$ – sedimentation velocity of a single particle of fraction II, m/s.

The balance of forces acting on a non-spherical particle is therefore as follows:

$$\sqrt{\left(\frac{\pi d_{\mathrm{II}e}^2}{4} \rho_l \frac{v_{\mathrm{II}o}^2}{2}\right)^2 \left(C_D^2 + C_M^2\right)} = (\rho_s - \rho_l)\, g \frac{\pi d_{\mathrm{II}e}^3}{6} (1 - \varepsilon). \tag{16}$$

In practice, determining the C_M coefficient for post-coagulation particles, whose shape is very diverse, is impossible. Determining the average rotational speed is also very difficult due

to the lack of simple measurement methods enabling such measurements. Hence, the most practical solution is to determine the total coefficient C_X which can be described by the following formula:

$$C_X = \sqrt{C_D^2 + C_M^2} \tag{17}$$

on an experimental path for the selected sedimentation process. This approach will cause the value of this coefficient to also include the impact of other phenomena accompanying non-linear sedimentation of particles, including the impact of particle collisions of fractions II and III.

The sedimentation velocity of a single particle can be then calculated by means of the following formula:

$$v_{\mathrm{II}0} = \sqrt{\frac{4(\rho_s - \rho_l) g d_{\mathrm{II}e}(1-\varepsilon_{\mathrm{I}})}{3\rho_l C_x}}. \tag{18}$$

The results of changes in sedimentation velocity depending on concentration are shown in Fig. 8:

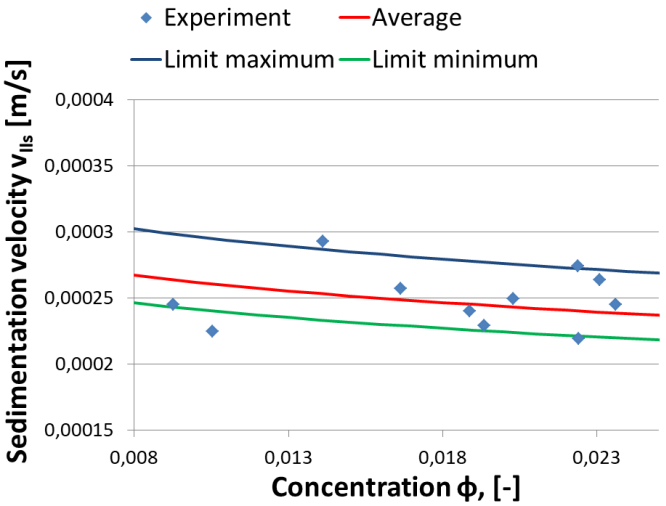

Fig. 8. Dependence of sedimentation velocity of monodisperse suspension of fraction II on the Φ concentration of this fraction, own study

Porous agglomerates are the third fraction of the polydisperse suspension being discussed. They are formed by non-spherical particles which have merged. The merging of non-spherical particles causes the formation of closed spaces within them, i.e. macropores, through which the liquid can flow during the particle's descent. This stabilizes the particle and causes it to drop in a straight line. A model similar to the one for spherical particles was used to describe the descent of this fraction, i.e. the force of gravity and the force of drag having the greatest influence on the sedimentation velocity of particles (Fig. 9)

The liquid flow through a network of macrochannels has been thoroughly described by models of liquid flow through a porous deposit. The Darcy–Weisbach equation describes the flow drag of porous materials. For a porous deposit with a network of [1] channels, the Darcy–Weisbach equation, called the Leva equation, needs to be modified [50]. Since the velocity and dimensions of the sedimentation particles are very small, the

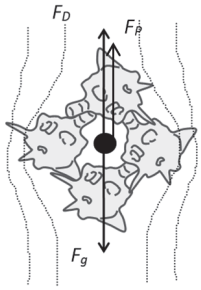

Fig. 9. Forces acting on an agglomerate

Reynolds number is a few orders smaller than 1. For Reynolds numbers smaller than 1, the Leva equation takes the form below:

$$\Delta p = \lambda \frac{L}{d_{\mathrm{II}e}} \frac{u^2 \rho}{2} \left(\frac{(1-\varepsilon)^{3-n}}{\varepsilon^3} \right) \varphi^{3-n}, \tag{19}$$

where: λ – linear coefficient of drag flow; u – linear velocity of fluid flow through the deposit, m/s; L – height of the deposit layer, m; $d_{\mathrm{II}e}$ – equivalent filling diameter, m.

The linear drag coefficient is calculated by the following formula [50]:

$$\lambda = \frac{400}{\mathrm{Re}}, \tag{20}$$

$$\lambda = \frac{400\eta_l}{v_{\mathrm{III}0} d_{\mathrm{III}e} \rho_l}, \tag{21}$$

where: $v_{\mathrm{III}0}$ – sedimentation velocity of a single particle of fraction III, m/s; $d_{\mathrm{III}e}$ – equivalent particle diameter of fraction III, m.

Therefore:

$$\Delta p = \frac{F_P}{A} = \lambda \frac{h}{d_{\mathrm{III}e}} \frac{\rho_l v_{\mathrm{III}0}^2}{2} \left(\frac{(1-\varepsilon_{\mathrm{I}})^2}{\varepsilon_{\mathrm{III}}^3} \right) \varphi^2, \tag{22}$$

where: $\varepsilon_{\mathrm{III}}$ – porosity of agglomerates; φ – shape factor.

By equating the volumes of a cylinder and a sphere, value h is obtained:

$$V_w = V_k, \tag{23}$$

$$\frac{\pi d_{\mathrm{III}e}^2}{4} h = \frac{\pi d_{\mathrm{III}e}^3}{6}, \tag{24}$$

then:

$$h = \frac{\pi d_{\mathrm{III}e}^3}{6} \frac{4}{\pi d_{\mathrm{III}e}^2} = \frac{2}{3} d_{\mathrm{III}e}, \tag{25}$$

therefore:

$$F_P = A \cdot \Delta p, \tag{26}$$

$$F_P = \frac{\pi d_{\mathrm{III}e}^2}{4} \frac{400\eta}{v_{\mathrm{III}0} d_{\mathrm{III}e} \rho_l} \frac{\frac{2}{3} d_{\mathrm{III}e}}{d_{\mathrm{II}e}} \frac{\rho_l v_{\mathrm{III}0}^2}{2} \left(\frac{(1-\varepsilon_{\mathrm{I}})^2}{\varepsilon_{\mathrm{III}}^3} \right) \varphi^2 \tag{27}$$

and after arranging the data:

$$F_P = \frac{\pi d_{\mathrm{IIIe}}^2 100\eta v_{\mathrm{IIIo}}}{3d_{\mathrm{IIe}}}\left(\frac{(1-\varepsilon_{\mathrm{I}})^2}{\varepsilon_{\mathrm{III}}^3}\right)\varphi^2, \tag{28}$$

$$F_G = gV_s(\rho_s-\rho_l)(1-\varepsilon), \tag{29}$$

$$F_G = g\frac{\pi d_{\mathrm{IIIe}}^3}{6}(\rho_s-\rho_l)(1-\varepsilon), \tag{30}$$

$$F_D = \frac{1}{2}C_D A_s \rho_l v_{\mathrm{IIIo}}^2, \tag{31}$$

where:

$$C_D = \frac{24}{\mathrm{Re}} = \frac{24\eta}{v_{\mathrm{IIIo}} d_{\mathrm{IIIe}}\rho_l}, \tag{32}$$

then:

$$F_D = \frac{1}{2}\frac{24\eta}{v_{\mathrm{IIIo}} d_{\mathrm{IIIe}}\rho_l}\frac{\pi d_{\mathrm{IIIe}}^2}{4}\rho_l v_{\mathrm{IIIo}}^2, \tag{33}$$

$$F_D = \pi d_{\mathrm{IIIe}} v_{\mathrm{IIIo}} 3\eta. \tag{34}$$

Thus, the balance of forces is as follows:

$$g\frac{\pi d_{\mathrm{IIIe}}^3}{6}(\rho_s-\rho_l)(1-\varepsilon) = \pi d_{\mathrm{IIIe}} v_{\mathrm{IIIo}} 3\eta_l + \frac{\pi d_{\mathrm{IIIe}}^2 100\eta v_{\mathrm{IIIo}}}{3d_{\mathrm{IIe}}}\left(\frac{(1-\varepsilon_{\mathrm{I}})^2}{\varepsilon_{\mathrm{III}}^3}\right)\varphi^2. \tag{35}$$

A formula for the particle sedimentation velocity can be derived from the balance of forces. After considering the relationship (21) for the drag coefficient and the formula for the Reynolds number, the formula for the sedimentation velocity of a single particle is calculated by the following formula:

$$v_{\mathrm{III0}} = \frac{d_{\mathrm{IIe}}(\rho_s-\rho_l)gd_{\mathrm{IIIe}}^2}{18\eta d_{\mathrm{IIe}} + d_{\mathrm{IIIe}}\cdot 200\eta_l}\frac{(1-\varepsilon_{\mathrm{I}})(1-\varepsilon_{\mathrm{III}})}{\left(\frac{(1-\varepsilon_{\mathrm{III}})^2}{\varepsilon_{\mathrm{III}}^3}\varphi^2\right)}. \tag{36}$$

The results of changes in sedimentation velocity depending on concentration are shown in Fig. 10.

The experimental results of particle sedimentation velocity were compared by calculating the sedimentation velocity of particles of similar size.

The results are presented in Table 1. Comparing the obtained results, we observe a strong correlation between the experimental and theoretical results. The differences in the results are slightly greater than 1%. This is the basis for the verification of the theoretical model that satisfactorily meets the requirements for theoretical sedimentation models. It can be used in the design of industrial devices that use the sedimentation process of polydisperse mixtures.

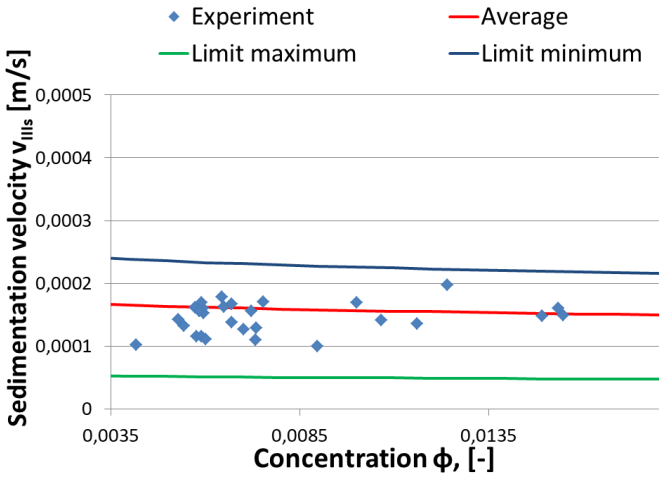

Fig. 10. Dependence of sedimentation velocity of monodisperse suspension of fraction III on the Φ concentration of this fraction, own study

Table 1
Comparison of sedimentation velocity results for monodisperse suspension of each fraction – comparison of experimental and theoretical results

Velocity v_s from the experiment (arithmetic average)	Velocity v_s from theoretical formulas (e.g. for $\Phi_o = 0.005$)
$v_{\mathrm{I}s} = 8.8934 \cdot 10^{-6}$ m/s	$v_{\mathrm{I}s} = 8.8525 \cdot 10^{-6}$ m/s
$v_{\mathrm{II}s} = 0.000247$	$v_{\mathrm{II}s} = 0.00028$
$v_{\mathrm{III}s} = 0.00015$ m/s	$v_{\mathrm{III}s} = 0.000166$ m/s

4.4. Flocculation modeling

There are different types of particles in the tested polydisperse suspension. Different in terms of size, shape and mass, which means that they fall at different velocities. Therefore, the sedimentation process is accompanied by a flocculation process. As a result of flocculation, inelastic collisions of various particles occur.

As a result of the inelastic collision of particles, their sedimentation velocity changes. In the case of agglomerates, collisions with smaller particles cause the volume of the agglomerate to increase and its sedimentation velocity becomes equal to the superposition of the velocities of the colliding particles. The higher the concentration of both fractions, the higher the probability of collisions. Therefore, the velocity correction resulting from collisions with particles representing other fractions can be described by the basic formula of fractions A and B [51, 52]:

$$v_{A-B} = \frac{m_A}{m_A+m_B}v_A + \frac{m_B}{m_A+m_B}v_B, \tag{37}$$

where m_A and m_B are the average masses of the particles from fractions A and B, and v_A, v_B stand for velocity of moving particle A and B.

In the case of coagulation, flocculation occurs simultaneously with sedimentation. This causes individual fractions in the selected volume to disappear at a different velocity than it

results from the sedimentation velocity [51]. The reason is the transformation of one fraction into another as a result of flocculation. Therefore, in the equations, the rate of disappearance of individual fractions in the selected volume should be supplemented with a flocculation model. At the beginning of the last century, Smoluchowski [52], while studying coagulation processes, formulated an equation for calculating the number of collisions of particles in monodisperse suspensions. On this basis, the number of particles that will remain without collisions in individual fractions after time t is:

$$N_{\mathrm{I}(n+1)} = \frac{N_0}{1+\dfrac{t}{T_{\mathrm{I}n}}}, \tag{38}$$

$$N_{\mathrm{II}(n+1)} = \frac{N_0}{1+\dfrac{t}{T_{\mathrm{II}n}}}, \tag{39}$$

$$N_{\mathrm{III}(n+1)} = \frac{N_0}{1+\dfrac{t}{T_{\mathrm{III}n}}}, \tag{40}$$

where $T_{\mathrm{I}n}$, $T_{\mathrm{II}n}$ and $T_{\mathrm{III}n}$ are the half-times of a given fraction of particles. These times can be calculated from:

$$T_{\mathrm{I}n} = \frac{1}{4\pi\delta D_{\mathrm{I}}}\frac{\pi d_{e\mathrm{I}}^3}{6\Phi_{\mathrm{I}n}V}, \tag{41}$$

$$T_{\mathrm{II}n} = \frac{1}{4\pi\delta D_{\mathrm{II}}}\frac{\pi d_{e\mathrm{II}}^3}{6\Phi_{\mathrm{II}n}V}, \tag{42}$$

$$T_{\mathrm{III}n} = \frac{1}{4\pi\delta D_{\mathrm{III}}}\frac{\pi d_{e\mathrm{III}}^3}{6\Phi_{\mathrm{III}n}V}, \tag{43}$$

where V is the total volume of the analyzed area.

The collision of the particles with each other causes the particles from fraction I to be transformed into particles of fraction II, while the particles of fraction II are transformed into fraction III. This changes the volume share of individual fractions. Only mutual collision of fraction III does not cause transition to the next fraction, yet larger particles are formed, which affects their sedimentation velocity.

Müller proposed the equation for calculating the number of particles for coagulation of the polydisperse suspension [52]. Based on its dependence, as a result of collisions of fraction I with fraction III, the number of particles of fraction I after time t will be:

$$N_{\mathrm{I,III}n+1} = \frac{N_{\mathrm{III}n}}{1+\dfrac{t}{T_{\mathrm{III}n}}} \cdot \frac{\dfrac{d_{e\mathrm{III}}}{d_{e\mathrm{I}}}}{\left(\dfrac{d_{e\mathrm{III}}}{d_{e\mathrm{I}}}\dfrac{N_{\mathrm{III}n}}{N_{\mathrm{I}n}}+1\right)\left(1+\dfrac{t}{T_{\mathrm{III}n}}\right)^{\frac{d_{e\mathrm{III}}}{d_{e\mathrm{I}}}}-1}. \tag{44}$$

As a result of collisions of fraction I with fraction II, the number of particles of fraction I after time t will be:

$$N_{\mathrm{I,II}n+1} = \frac{N_{\mathrm{II}n}}{1+\dfrac{t}{T_{\mathrm{II}n}}} \cdot \frac{\dfrac{d_{e\mathrm{II}}}{d_{e\mathrm{I}}}}{\left(\dfrac{d_{e\mathrm{II}}}{d_{e\mathrm{I}}}\dfrac{N_{\mathrm{II}n}}{N_{\mathrm{I}n}}+1\right)\left(1+\dfrac{t}{T_{\mathrm{II}n}}\right)^{\frac{d_{e\mathrm{II}}}{d_{e\mathrm{I}}}}-1}. \tag{45}$$

As a result of collisions of fraction II with fraction III, the number of particles of fraction II after time t will be:

$$N_{\mathrm{II,III}n+1} = \frac{N_{\mathrm{III}n}}{1+\dfrac{t}{T_{\mathrm{III}n}}} \cdot \frac{\dfrac{d_{e\mathrm{III}}}{d_{e\mathrm{II}}}}{\left(\dfrac{d_{e\mathrm{III}}}{d_{e\mathrm{II}}}\dfrac{N_{\mathrm{III}n}}{N_{\mathrm{II}n}}+1\right)\left(1+\dfrac{t}{T_{\mathrm{III}n}}\right)^{\frac{d_{e\mathrm{III}}}{d_{e\mathrm{II}}}}-1}. \tag{46}$$

The above considerations constitute the basis for calculating the volume shares of individual fractions in the analyzed volume. After time t, the concentrations of individual fractions are calculated according to the following formulas:

$$\Phi_{\mathrm{I}(n+1)} = \left(1-\frac{A\,v_{\mathrm{I}so}t}{V}\right)\Phi_{\mathrm{I}n} - \frac{N_{\mathrm{I}(n+1)}}{N_{\mathrm{I}n}}\Phi_{\mathrm{I}n} - \frac{N_{\mathrm{I,III}(n+1)}}{N_{\mathrm{I}n}}\Phi_{\mathrm{I}n} - \frac{N_{\mathrm{I,II}(n+1)}}{N_{\mathrm{I}n}}\Phi_{\mathrm{I}n}, \tag{47}$$

$$\Phi_{\mathrm{II}(n+1)} = \left(1-\frac{A\,v_{\mathrm{II-I}}t}{V}\right)\Phi_{\mathrm{II}n} - \frac{N_{\mathrm{II}(n+1)}}{N_{\mathrm{II}n}}\Phi_{\mathrm{II}n} + \frac{N_{\mathrm{I},(n+1)}}{N_{\mathrm{I}n}}\Phi_{\mathrm{I}n} + \frac{N_{\mathrm{I,II}(n+1)}}{N_{\mathrm{I}n}}\Phi_{\mathrm{I}n} - \frac{N_{\mathrm{II,III}(n+1)}}{N_{\mathrm{II}n}}\Phi_{\mathrm{II}n}, \tag{48}$$

$$\Phi_{\mathrm{III}(n+1)} = \left(1-\frac{A(v_{\mathrm{III-I}}+v_{\mathrm{III-II}})t}{V}\right)\Phi_{\mathrm{III}n} + \frac{N_{\mathrm{II}(n+1)}}{N_{\mathrm{II}n}}\Phi_{\mathrm{II}n} + \frac{N_{\mathrm{II,III}(n+1)}}{N_{\mathrm{II}n}}\Phi_{\mathrm{II}n} + \frac{N_{\mathrm{I,III}(n+1)}}{N_{\mathrm{I}n}}\Phi_{\mathrm{I}n}. \tag{49}$$

Equation (47), describing the reduction of the concentration of phase I, consists of the term describing the reduction of the proportion, as a result of sedimentation of particles, as well as the flotation terms of phase I particles and the interaction with phases II and III. Equation (48) takes into account the increase in concentration through the formation of additional particles as a result of mutual collision of fraction II particles, and the collision of fraction I with fraction II, which causes an increase in the volume of fraction II particles. In turn, the loss of fraction III is caused only by its falling, while fraction II particles are added by means of mutual flotation and through collisions of fraction III particles with fraction I and II.

As a consequence of the collision of two particles, one particle is formed with a mass equal to the sum of both, and its movement velocity must be corrected in accordance with equation (37). Therefore, various formulas were derived that consider the mutual collisions of particles of individual fractions.

These formulas also concern the flocking of particles of different fractions.

In this case, the formula for the velocity of a particle after the collision of fraction II with fraction I and for the probability of collision will be the following:

$$v_{\text{II-I}} = \left(\frac{d_{e\text{I}}^3 (1-\varepsilon_{\text{I}})}{d_{e\text{I}}^3 (1-\varepsilon_{\text{I}}) + d_{e\text{II}}^3 (1-\varepsilon_{\text{II}})} v_{\text{I}so} + \frac{d_{e\text{II}}^3 (1-\varepsilon_{\text{II}})}{d_{e\text{I}}^3 (1-\varepsilon_{\text{I}}) + d_{e\text{II}}^3 (1-\varepsilon_{\text{II}})} v_{\text{II}so} \right) \left(\frac{6\Phi_{\text{I}n} V}{\pi d_{e\text{I}}^3} - N_{\text{I,II}n} \right) \frac{\pi d_{e\text{II}}^3}{6\Phi_{\text{II}n} V}. \tag{50}$$

Similarly, you can calculate the corrected motion velocity of fraction III particles colliding with fraction II:

$$v_{\text{III-II}} = \left(\frac{d_{e\text{II}}^3 (1-\varepsilon_{\text{II}})}{d_{e\text{II}}^3 (1-\varepsilon_{\text{II}}) + d_{e\text{III}}^3 (1-\varepsilon_{\text{III}})} v_{\text{II}so} + \frac{d_{e\text{III}}^3 (1-\varepsilon_{\text{III}})}{d_{e\text{II}}^3 (1-\varepsilon_{\text{II}}) + d_{e\text{III}}^3 (1-\varepsilon_{\text{III}n})} v_{\text{III}so} \right) \left(\frac{6\Phi_{\text{II}n} V}{\pi d_{e\text{II}}^3} - N_{\text{II,III}n} \right) \frac{\pi d_{e\text{III}}^3}{6\Phi_{\text{III}n} V}, \tag{51}$$

where as a result of collisions of fraction III with fraction I the equation of velocity has the form below:

$$v_{\text{III-I}} = \left(\frac{d_{e\text{I}}^3 (1-\varepsilon_{\text{I}})}{d_{e\text{I}}^3 (1-\varepsilon_{\text{I}}) + d_{e\text{III}}^3 (1-\varepsilon_{\text{III}})} v_{\text{I}so} + \frac{d_{e\text{III}}^3 (1-\varepsilon_{\text{III}})}{d_{e\text{I}}^3 (1-\varepsilon_{\text{I}}) + d_{e\text{III}}^3 (1-\varepsilon_{\text{III}})} v_{\text{III}so} \right) \left(\frac{6\Phi_{\text{I}n} V}{\pi d_{e\text{I}}^3} - N_{\text{I,III}n} \right) \frac{\pi d_{e\text{III}}^3}{6\Phi_{\text{III}n} V}. \tag{52}$$

The numbers $N_{\text{II,I}}$, $N_{\text{III,I}}$ and $N_{\text{III,II}}$ denote the number of particles that remained after the collision time, the number of particles that stood for the probability of the number of particle collisions that will occur during the coagulation process for suspensions of a certain concentration.

5. ALGORITHM

The described model of the sedimentation process allows for iterative simulation of the process with a fixed time step. The result of the simulation is the concentration of individual fractions. This allows to calculate the share for any time, which can provide valuable information when designing equipment and the sedimentation process. It is not beneficial to set a too narrow time step. It should be chosen equivalently to all iterative models. If the changes in subsequent time steps are small, causing the algorithm to lose convergence, then it should be increased. Similar criteria are used for large time steps.

An experiment was carried out where the following results were obtained for the parameters: the liquid density and suspension density are known $\rho_L = 997$ kg/m^3 and $\rho_S = 2127$ kg/m^3 and sediment porosity $1-\varepsilon_{\text{I}} = 0.72$, porosity of agglomerates $1-\varepsilon_{\text{III}} = 0.62$, equivalent diameter of the particles $d_{\text{I}e} = 0.0000047$ m, $d_{\text{II}e} = 0.000057$ m, $d_{\text{III}e} = 0.0002$ m.

The algorithm calculation begins with determining the initial conditions at time $t = 0$ s. This is the moment when the sedimentation process begins. At this time, it is assumed that the entire analyzed volume V contains a homogeneous mixture consisting only of fraction I with concentration $\Phi_{\text{I}o}$. Fraction II and III volume shares are $\Phi_{\text{II}o} = 0$ and $\Phi_{\text{III}o} = 0$ with porosity $\varepsilon_{\text{II}} = 0$ and $\varepsilon_{\text{III}} = 0$.

The process of coagulation is used for water treatment. After adding the coagulant, the binding of iron II to iron III particles begins for the first time. This produces small particles and fractions in the entire volume of the liquid. In subsequent stages of the process, fraction II is formed through flocculation of fraction I, with simultaneous fall of particles of fraction I. In turn, fraction III is formed as a result of flocculation of fraction II. During the process, all fractions sedimentate with different velocities, and at the same time particles collide, which causes a change in their velocity and weight of the particles.

In the **first time step**, the average sedimentation velocity of a single particle is calculated using formula (12). Next, the suspension sedimentation velocity is calculated taking into account the movement of the liquid on the basis of formula (4). The liquid velocity occurring in the formula is calculated on the basis of relation (7), where Φ_z (formula (8)), i.e. of all phases, is equal to Φ_{I}, since at the beginning of the process only fraction I occurs, and the volume shares Φ_{II} and Φ_{III} are equal to 0. Such calculated velocity of sedimentation $v_{\text{I}so}$ is used to calculate the sedimentation velocity of fraction I $v_{\text{I}s}$ using formula (1). The number of particles left over time t_n due to flocculation is calculated from formula (38).

A new concentration of fraction I is then calculated after time t_n according to formula (47). Because in the first step there is no fraction II and III, hence the values $N_{\text{I,II}(n+1)}$, $N_{\text{I,III}(n+1)}$ and $N_{\text{II,III}(n+1)}$ are equal to zero.

The number of particles that as a result of flocculation has passed from fraction I to fraction II constitutes the basis for calculating the number of particles of fraction II:

$$N_{\text{II}fn} = \frac{N_{\text{I}n} - N_{\text{I}(n+1)}}{2}. \tag{53}$$

Based on the number of fraction II particles and their concentration, the equivalent diameter of fraction II particles is calculated:

$$d_{\text{II}e} = \frac{6\Phi_{\text{I,II}(n+1)} V}{\pi N_{\text{II}fn}}. \tag{54}$$

In the **second time step**, the sedimentation velocity of fraction II particles is calculated based on formula (18). In turn, sedimentation velocities of fractions I and II are calculated from formulas (5) and (2). For fraction II, the sedimentation velocity is corrected due to the collisions of particles from fraction II with particles of fraction I based on formula (50).

The number of particles remaining in fractions I and II after the flocculation process is calculated according to formulas (38) and (39). On this basis, concentration Φ for fractions I, II and III

is calculated using formulas (47), (48) and (49), assuming that $N_{\mathrm{II,III}(n+1)}$ is equal to zero. The particle numbers of fractions II and III are calculated then:

$$N_{\mathrm{II}f(n+1)} = N_{\mathrm{II}(n+1)} + \frac{N_{\mathrm{I}n} - N_{\mathrm{I}(n+1)}}{2} - \frac{A v_{\mathrm{IIz}\mathrm{I}} t_n}{V} N_{\mathrm{II}n}, \quad (55)$$

$$N_{\mathrm{III}fn} = \frac{N_{\mathrm{II}n} - N_{\mathrm{II}(n+1)}}{2}. \quad (56)$$

The particle numbers are used to calculate the equivalent diameters for fraction II particles using formula (54), while for fraction III particles the number is:

$$d_{\mathrm{III}e} = \frac{6\Phi_{\mathrm{III}(n+1)} V}{\varepsilon_{\mathrm{III}} \pi N_{\mathrm{III}fn}}. \quad (57)$$

All three fractions are already taking part in the **third time step**. The sedimentation velocities of the particles of each fraction are calculated according to formulas (12), (18) and (36). Based on this, fraction I, II and III sedimentation velocities are calculated based on formulas (4)–(6). Then, for fraction II, the sedimentation velocity is corrected due to the collision of the particles with the particles of fraction I by means of formula (50), while the sedimentation velocity of fraction III is the resultant of the velocities of collisions with the particles of fractions I and II calculated on the basis of formulas (52) and (51). The value of fraction III sedimentation velocity is described by the following formula:

$$v_{\mathrm{III}} = \frac{v_{\mathrm{III-I}} + v_{\mathrm{III-II}}}{2}. \quad (58)$$

The number of particles remaining in fractions I, II and III after the flocculation process is calculated from formulas (38), (39) and (40). On this basis, the concentration of fractions I, II and III are calculated from formulas (47), (48) and (49). The particle numbers of fraction II are then calculated by formula (55), and for fraction III by the formula below:

$$N_{\mathrm{III}f(n+1)} = N_{\mathrm{III}(n+1)} + \frac{N_{\mathrm{II}n} - N_{\mathrm{II}(n+1)}}{2} - \frac{A\, v_{\mathrm{IIIz}} t_n}{V} N_{\mathrm{III}n}. \quad (59)$$

Equivalent diameters for particles of fractions II and III are calculated according to formulas (54) and (57).

In the next time steps, the calculations from the third step are repeated, and similarly, the next concentrations of individual fractions in the analyzed volume are calculated for successive intervals.

6. CONCLUSIONS

The model described above assumes that the particles flocculate during their sedimentation, which accelerates the process. The models available in literature often do not take particle shape into account, while some models assume variable densities [53–55]. In this model, the density of particles is constant, which is irrelevant in this case, and the model developed fits all flocculation processes as it takes into consideration intermolecular interactions. A model comprising the shape of particles for individual fractions and mutual interactions between particles has been proposed. Since it is merely a theoretical proposal, the model would require experimental verification, which will be the subject of further research and articles. The conclusion is that the algorithm can be used in the water purification process. Often, the process of chemical water treatment consists in adding a coagulant, which causes the formation of a postcoagulation suspension, which sedimentates, causing the separation of fractions. Due to the need to design such devices, a mathematical description of the sedimentation process of polydisperse suspensions is highly necessary. This article may become a valuable supplement to the current knowledge.

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