Simulation of Solids Flocculation by CFD-PBM Method

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Abstract

In alumina production of great importance is separation of suspension into liquid and solid components. Settling rate depends significantly on the size of solid particles; therefore, one of the ways to raise efficiency of a thickener is to enlarge the effective size of solid particles by means of reagents – flocculants. Flocculation process is accompanied by simultaneous growth and breakage of agglomerates under the influence of turbulent forces. Hydrodynamic conditions under which it proceeds have significant effect on dynamics of the process. In the paper, a CFD PBM method is considered comprising solution of population equation balance, describing a process of agglomeration and breakage of flocs in the environment of computational fluid dynamics. In the paper laws of agglomeration and breakage of flocs are provided, a laboratory installation and technique enabling to determine parameters of laws of flocs agglomeration and breakage is described, examples of thickeners simulation by CFD-PBM method are given. The proposed CFD-PBM method allows to predict growth dynamics of flocs depending on design and hydrodynamic features of the thickener and determine measures to increase productivity and improve process characteristics of thickeners.

Keywords: thickener, flocculation, CFD, PBM.

1. Flocculation

Today chemical reagents, such as flocculants, are widely used in a thickening area of alumina production. The process of flocculation is accompanied by merging of particles of slurry in agglomerates. Solids, integrated in a group, obtain raised settling rate that enables to increase productivity or to improve process characteristic of thickeners.

The result of flocculation is affected by a set of factors such as: properties of particles surface, molecular weight of flocculant, type of flocculant polymeric chain, method of flocculant feeding, properties of liquid phase of suspension and others, but of most importance are intensity and period of mixing of suspension that are investigated in this work

Flocs are essentially complex porous structures consisting of groups of particles. Kranenburg suggested to consider that a floccule consists of similar structures, i.e. is a fractal [1]. The structure of Flocs is characterized by fractal dimension D_f, which does not coincide with dimension of space and can acquire any values from 1 to 3. Values close to 1 correspond to thin thread, D_f =3 value corresponds to a continuous (nonporous) sphere (Figure 1). Introduction of a concept of fractal dimension allowed to connect the size of a floccule with its sedimentation rate.

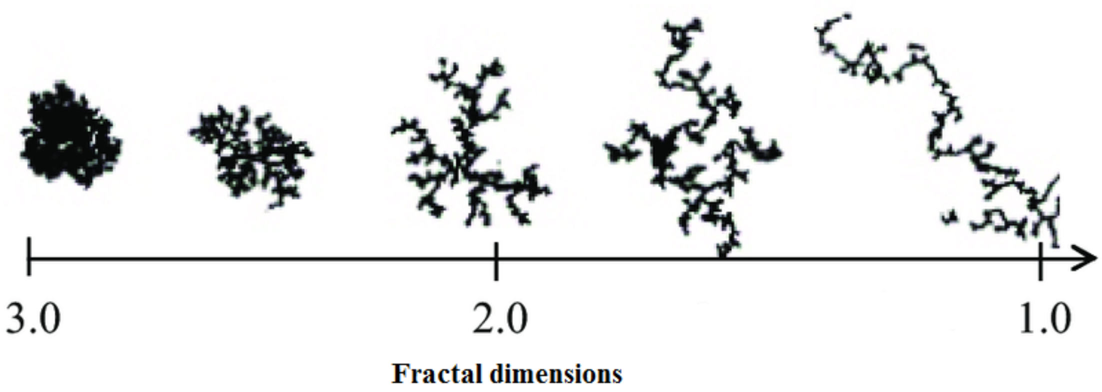


Figure 1. Flocs of various fractal dimension.

2. Settling Rate of Flocs

Settling rate of spherical particles at small Reynolds numbers (Re <0.2) is described by Richardson-Zacky law which considers a factor of particles concentration [2]:

$$V_s = \frac{d_s^2 g(\rho_s-\rho_l)}{18\mu}(1-\varphi)^{4,65} \qquad (1)$$

where:

Vs	settling rate of spherical particles, m/s
d_s	diameter of a particle, m
ρ_s	density of particles, kg/m^3
ρ_l	density of liquid, kg/m^3
μ	dynamic viscosity of liquid, Pa·s
g	gravitational acceleration, m/s^2
φ	particle volume fraction, m^3/m^3

Taking into account fractal structure of a floccule the law will be transformed to the equation, published in [3]:

$$V_s = \frac{\overline{d_{agg}^2}\, g(\rho_s-\rho_l) K_p \left(\frac{d_{agg}}{d_p}\right)^{D_f-3}}{18\mu}\left(1-\frac{\varphi}{K_p}\left(\frac{d_{agg}}{d_p}\right)^{3-D_f}\right)^{4,65} \qquad (2)$$

where:

$\overline{d_{agg}}$	average diameter of a floccule, m
$\overline{d_p}$	average diameter of initial particle, n
D_f	fractal dimension of a floccule
K_p	packing limit

3. Model of Population Balance. Smoluchowski Equation

Flocculation is essentially a process of particles aggregation in flocs accompanied by simultaneous growth and breakage for the account of shear stress in liquid. It is a dynamic process with the rate depending on properties of particles, flocculant and mixing conditions.

Shear stress provides thorough mixing and high probability of collisions between particles and, therefore, rapid growth of flocs. At the beginning of flocculation process particles quickly aggregate, however, when flocs become larger, their susceptibility to breakage increases. In a while, a steady state between growth and breakage of flocs is reached, and flocs size distribution does not change over time any more.

General approach to the description of dynamics of flocculation process comprises combination of the law of probability of collisions of particles causing their coagulation and the law of breakage of particles within the equation of population balance. This equation allowing to simulate dynamics of change of diameter of particles in the course of coagulation was introduced for the first time by Marian Smoluchowski [4]. Smoluchowski's equation considering effects of coagulation and fragmentation (breakage) of particles takes the form:

$$\frac{dn_i}{dt} = \frac{1}{2}\sum\nolimits_{j+k=i} \alpha\beta(u_j, u_k) n_j n_k - n_i \sum\nolimits_{k=1}^{max} \alpha\beta(u_k, u_i) n_k - S_i n_i + \sum\nolimits_{j=i}^{max} \gamma_{i,j} S_j n_j \tag{3}$$

where:

n_i number density of flocs of the size i, m^{-3}

t time, s

α capture efficiency factor or share of the collisions leading to coagulation;

$\beta(u_j, u_k)$ frequency of collisions of particles having volumes u_j anf u_k, m^3/s

S_i frequency of breakage of flocs of the size i, c^{-1}

$\gamma_{i,j}$ function of distribution of fragments defining volume fraction of fragments of size *i* arriving from flocs of size *j*.

Index *max* represents the largest size of particles formed at breakage of flocs of size *i*. The first summation in the right hand side of the equation 3 is formation of particles consisting of *i* primary particles at collision of smaller particles of *j* and *k* sizes. The second member in the right hand side of the equation designates the loss of particles of *i* size in collision with particles of any other size. The third member in the right hand side of the equation describes the loss of particles of *i* size due to their breakage, and the fourth member in the right hand side of the equation describes formation of particles of *i* size by breakage of larger particles

3.1. Agglomeration and Breakage Kernel

Agglomeration and breakage kernel describe physics of the process of flocculation and are the most important equations in the model of population balance**.** Frequency of collisions for coagulation of particles caused by turbulent shear stress was offered by Saffman and Turner [5].

$$\beta(V_i, V_j) = 0{,}31G\alpha(V_i^{\frac{1}{3}} + V_j^{\frac{1}{3}})^3 \tag{4}$$

where:

G Shear rate, c^{-1}

α capture efficiency factor

In [6] agglomeration kernel was complemented with capture efficiency factor that determines a share of collisions leading to coagulation of particles. Capture efficiency factor is set by time dependence that allows to consider degradation effect of the flocculant or loss of activity due to a gap or regrouping of polymeric structure:

$$\alpha = Ce^{-t/D} \tag{5}$$

where:

C initial capture efficiency factor

t time, c
D parameter determining the rate of flocculant degradation

The nucleus of flocs breakage used in the paper was proposed by Kapur's function from the volume of flocs [7]:

$$S_i = AV_i^a \tag{6}$$

where:
a equal to 1/3
A factor of flocs breakage rate

Breakage rate is proportional to diameter of flocs. The factor of flocs breakage rate depends on shear rate by dependence:

$$A = PG^Y \tag{7}$$

where:
Y constant, inversely proportional to Flocs strength
P proportionality constant that is determined experimentally

4. Simulation of Flocculation by CFD-PBM Method

For setting and verification of mathematical model of slurry flocculation process, laboratory investigations of impact of conditions of slurry and flocculant mixing on slurry settling rate were performed. Investigations were conducted on a slurry of nepheline mud of JSC RUSAL Achinsk. At various periods and rotation rate of a mixer the slurry was mixed with flocculant, then settling test of the flocculated slurry was carried out. The laboratory unit for mixing of slurry and flocculant is presented in Figure 2.

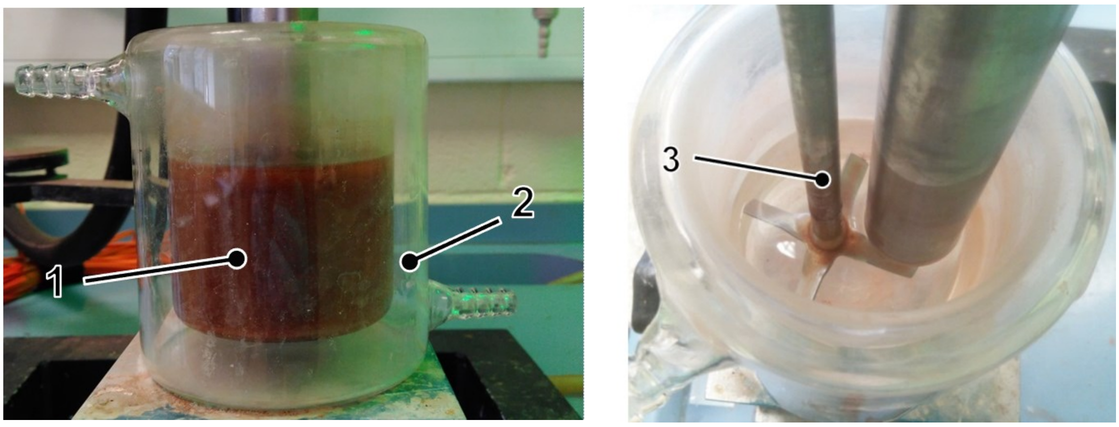


Figure 2. The laboratory unit for mixing of slurry and flocculant
1 – slurry, 2 – container, 3 – impeller

In [8, 9] the size of flocs was determined by means of measuring systems FBRM (Focused Beam Reflectance Measurement). The advantage of FBRM is that the device allows to assess sizes of particles in a continuous mode. The drawback of the device is that at the output, it gives distribution of lengths of chords of particles and for determination an average diameter of floccule, additional mathematical processing is required which is complicated due to nonsphericity of flocs. In our work, a method is proposed of assessment of flocs sizes by the results of settling tests which does not require the use of expensive measuring devices. At the second stage, parameters of agglomeration and breakage models of flocs were determined, using methods of computational fluid dynamics (CFD) with population balance module (PBM).

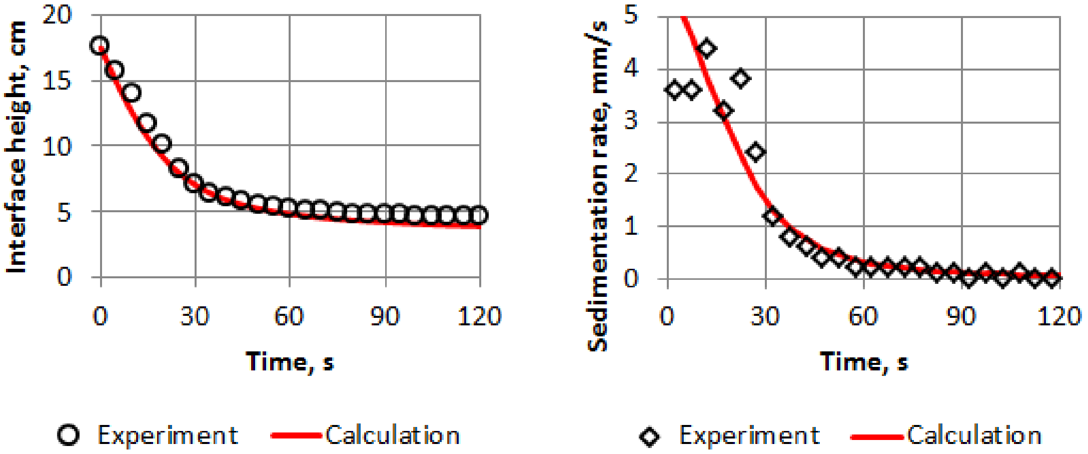


Figure 3. Calculated and experimental data of the settling test.

In figure 4 a geometrical model of a laboratory unit is presented for mixing slurry with flocculant and its grid consisting of 1.75 million cells.

Multiphase liquid was simulated by Euler-Euler approach of the *Mixture* model. Mixing was simulated in a stationary statement by the method of *Multiple Reference Frame*. Distribution of the solid phase by fractions was set by means of a homogeneous discrete population balance method (*PBM*). In calculations, 41 fractions (bin) having minimum diameter 1 µm and double change of interval of particles volume was used. Densities of liquid and solid phases of the slurry were 1134 and 3134 kg/m^3 respectively. Viscosity of the liquid phase was 0.3 cPs. Calculation of flocculation process by PBM method was performed in non-stationary statement, preceded by stabilized distribution of rates and phases of slurry in the volume of the beaker. As a result of calculation dynamics in the change of slurry particles diameter depending on time as well as shear rate created by the mixing device was determined.

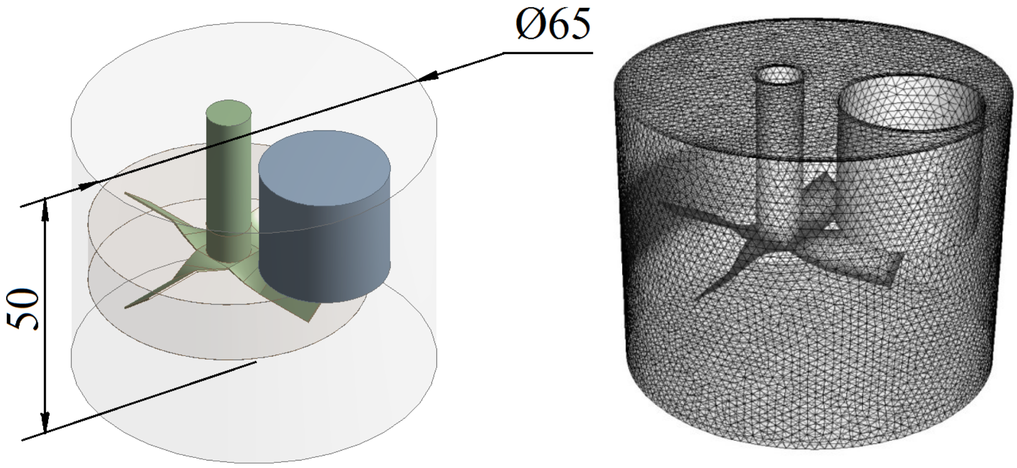


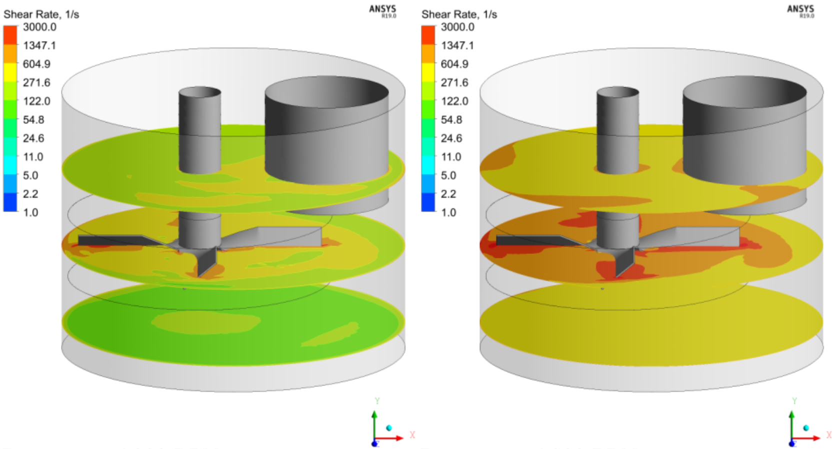
Figure 4. Geometry and computational grid of the unit for mixing slurry with flocculant.

The obtained distributions of shear rates at various rotation rates of the mixer are presented in Figure 5. PBM agglomeration model factors were selected by approximation of calculated values of flocs diameter to the experimental ones by the least squares method (Table 1). Factors were used of PBM breakage model from [10]. By the results of simulation, the error of determination of average diameter of flocs did not exceed 15 % (Table 2).

The curves of changing of flocs size depending on period of mixing with flocculant under various conditions of mixing are presented in Figure 6. The diagram clearly demonstrates zones of growth and breakage of flocs.

Table 1. Factors of kernel of PBM agglomeration and breakage.

Factor	Agglomeration kernel	Breakage kernel
D_f	2,300	
C	0,13	-
D	60	-
P	-	1,23
Y	-	1,88



Rotate speed 200 RPM

Rotate speed 300 RPM

Figure 5. Contour field of shear rates distribution in the beaker at various rotation rates of the mixer (logarithmic scale).

Table 2. Average diameters of flocs obtained by calculations and experimentally.

Rotation rate of the mixer, rpm	Av. shear rate, c^{-1}	mixing time, s	Diameter, µm		Relative error, %
			Experimental	Calculated	
100	80	10	98	83	15
200	250	10	112	126	12
		20	114	124	9
300	450	10	110	116	5
		20	100	95	5
		40	75	64	15

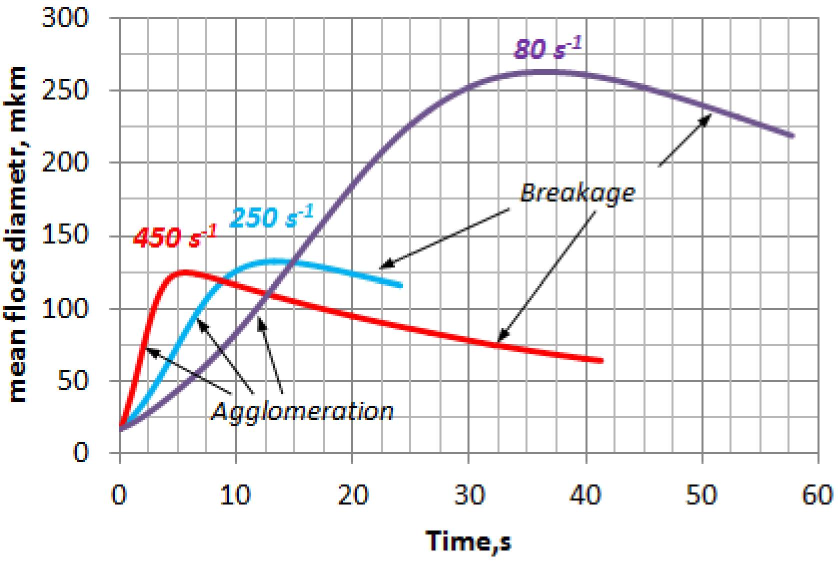


Figure 6. Diagram of flocs size changing depending on period of mixing with flocculant.

Figure 6 demonstrates the way of population balance model PBM work in calculation:

- at the initial stage of mixing of slurry with flocs agglomeration processes prevail over breakage, active growth of flocs is observed, and the higher is shear rate in the volume, the higher is growth rate of flocs;
- after achievement of a certain size, breakage of flocs occurs, the higher is shear rate, the earlier starts this process;
- high shear rates (exceeding 100 c^{-1}) leads to early breakage of flocs preventing gaining of larger sizes.

5. Simulation of Feeding Unit of Sodium Carbonate Thickener

Mixing of slurry with a flocculant by means of a mixing device in a beaker takes place in a wide range of shear rates that brings inaccuracies in the study of shear rates impact on aggregation and breakage rate of flocs. A laboratory bench to study the process of settling of polydisperse slurry (further SPS) was developed to improve the accuracy of physical simulation of the process of slurry flocculation, where mixing of slurry with flocculant occurs in a vessel with Taylor flow, and settling of slurry takes place in a graduated column.

Figure 7. General view of SPS.

At SPS, laboratory investigations of sodium carbonate slurry flocculation were conducted. Liquid phase of slurry is a strong soda-alkaline liquor, solid phase – berkeit ($2Na_2SO_4 \times Na_2CO_3$) and sodium carbonate monohydrate ($Na_2CO_3 \times H_2O$).

Analysis of the results of flocculation slurry tests showed that the best settling rate of the slurry was achieved at long-lasting mixing of slurry with flocculant (51 seconds) under conditions of minor shear rates, below 100 c^{-1}. The results of physical simulation of sodium carbonate slurry flocculation process formed a basis for mathematical simulation and development of sodium carbonate thickener unit by CFD-PBM method for RUSAL Krasnoturyinsk alumina refinery. Mathematical simulation allowed to study slurry flows in feed wells of various designs and to estimate their impact on the size of flocs at the exit from the feed well.

An option including cylindrical feed wells with one tangential input and various constructions inside the well in a form of shelves and baffles of various forms were considered. In Figures 8 and 9 distributions of shear rate in the feed wells of the thickener of various configurations and their impact on particle size distribution of flocs at the exit from the feed well are presented. By the results of simulation, the optimum size of the feed well and the construct of elements in the well were determined.

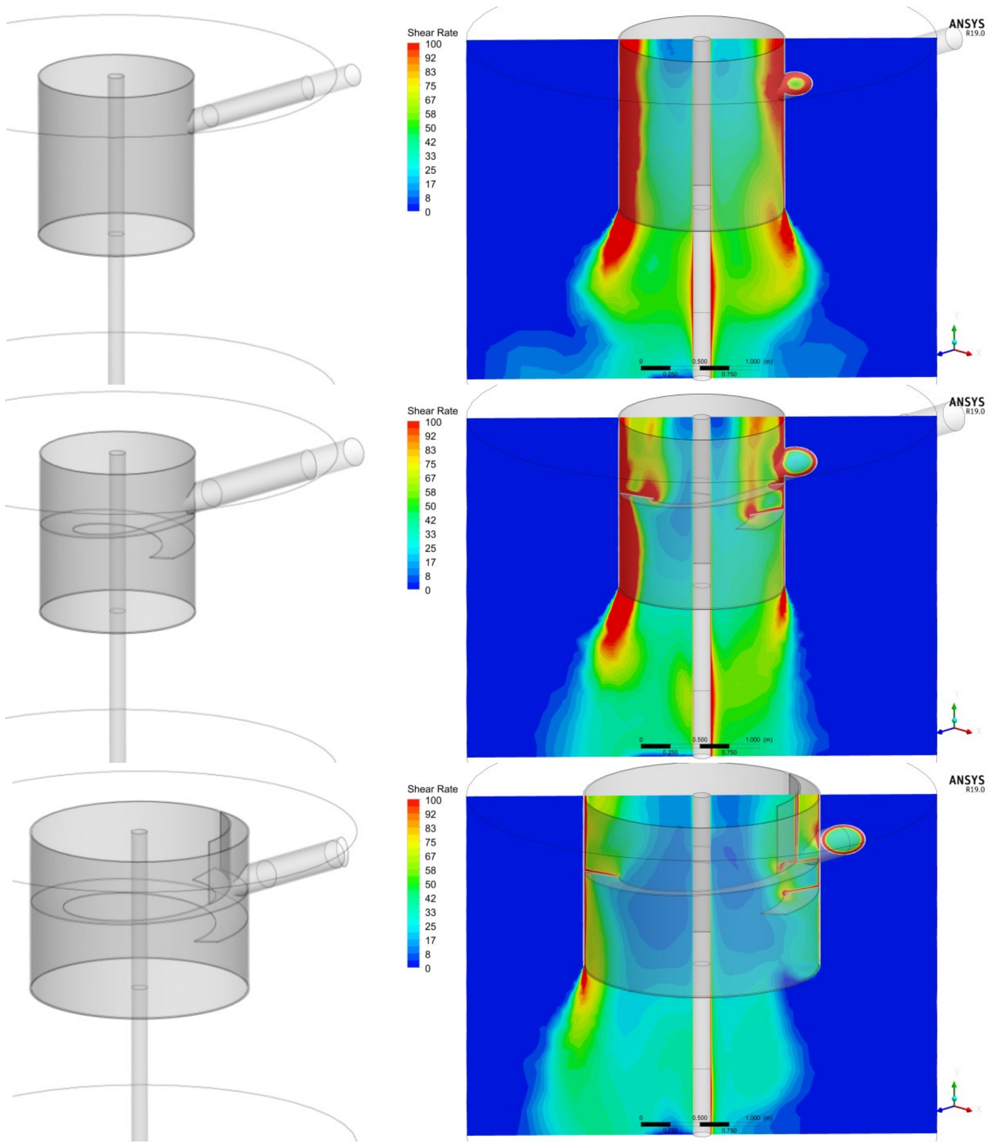


Figure 8. Geometry and distribution of shear rates in feed wells of sodium carbonate thickener of various configurations.

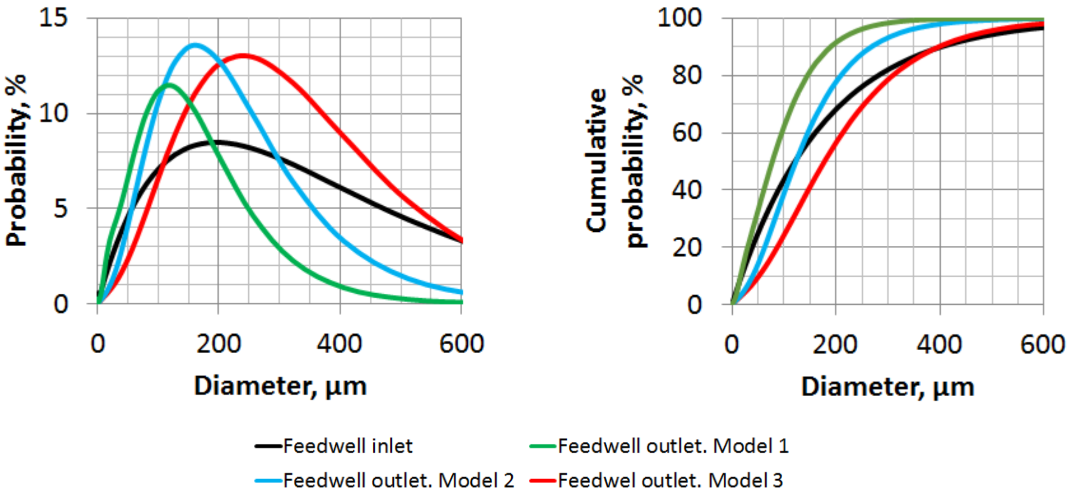


Figure 9. Particle size distribution of flocs in models of feeding unit of thickener.

6. Conclusion

In the paper, the CFD-PBM method is described and tested for description of dynamics of slurry motion, distribution of a solid phase and kinetics of flocculation in thickening devices, such as: red mud thickeners and washers, sodium carbonate thickeners. Physical simulation of slurry flocculation process of nepheline mud is carried out, a method is proposed for determination of an average size of flocs by means of settling test, setup of parameters of kernel agglomeration and breakage of population balance model of nepheline mud is made enabling to reach an error in determination of average diameter of flocs not exceeding 15%. CFD-PBM method was used in developing a new design of feed well of sodium carbonate thickener at RUSAL Krasnoturyinsk alumina refinery. Simulation of gravitational thickeners by CFD-PBM method makes it possible to determine measures enabling to raise productivity or to improve performance of the device.

7. References

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