

Effect of dispersion degree and colloidal suspension concentration on the coagulation process – a computer simulation

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Received 7 October 2019; Accepted 2 May 2020

ABSTRACT

This paper presents the findings of a study on the impact of the sol dispersion degree and concentration on the kinetics of coagulation–flocculation of a colloidal suspension. The study was conducted with original ZB2 computer software, which simulates the processes of coagulation–flocculation of wastewater suspension. The software was created based on long-term studies of the processes of coagulation and electrocoagulation conducted with natural and model wastewater. The results of simulation studies were tested by conventional rate equations for first and second-order reactions. The simulated coagulation process rate was found to be consistent with the kinetic equations of first and second-order reactions. The sol concentration was found to have a significant effect on the colloidal system destabilization time. An increase in the sol concentration brought about an increase in the colloidal suspension coagulation–flocculation rate. The simulated coagulation rate depended on the sol dispersion degree and increased with an increasing ratio of sol particle radius to the coagulant particle radius. The impact of the sol concentration on the colloidal system destabilization time decreased with the increasing size of the sol particles.

Keywords: Colloidal suspension; Coagulation rate; Computer simulation

1. Introduction

Solid contaminants are usually present in water and wastewater as colloids which – owing to their size – create stable suspensions. The coagulation process is one of the most effective methods for eliminating these types of contaminants [1,2]. Coagulation/flocculation plays a dominant role in many water and wastewater treatment systems. A properly proceeded coagulation process ensures not only high efficiency of removal of colloids and suspensions difficult to sediment but also associated impurities. Coagulation is defined as a process of aggregation of colloidal particles and fine suspensions to larger agglomerates, which can be later removed by sedimentation, flotation, and filtration [3]. The coagulation process is a two-step process. The first

step takes place immediately after the destabilizing factor is added and it consists of chemical reactions and physical interactions, which involve, among others, decreasing the electrokinetic potential of colloidal particles, dehydration, and the oxidation of protecting colloids. The second step, which lasts much longer, involves particle agglomeration, called flocculation, in which transport and collisions of particles result in the formation of flocs, which can be removed effectively by sedimentation/flotation and filtration.

Coagulation–flocculation is a kinetic process that runs at a lower or higher rate; the coagulation efficiency, the properties of post-coagulation structures, and those formed by condensation depend largely on the aggregation rate [4–6]. The coagulation kinetics are affected by a range of chemical and physical factors. The chemical factors include

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concentration and type of contaminants in water, pH, and chemical composition of water and the type of coagulant. The physical factors affecting the coagulation kinetics include temperature, as well as mixing time and speed. Colloid destabilization during coagulation is the result of several mechanisms, which largely depend on the factors mentioned above, especially the type and concentration of colloids removed, pH value, type, and dose of the used coagulant. These mechanisms are • electrostatic destabilization (charge neutralization), double layer compression, bridging, and sweep [7]. Due to the complex interdependence of many factors affecting the course and effectiveness of the coagulation process, research on this process and its improvement are necessary. Researchers' attention is focused on the introduction of new coagulants, for example, modified composite coagulants, which are becoming more and more complex in terms of composition, but also more effective in comparison to traditionally used reagents [8], in the study of hybrid processes combining coagulation with other purification methods [9]. Research is ongoing on coagulant dose control regimens because the basic procedural problem of wastewater treatment by chemical coagulation is the choice of coagulant and precise determination of its optimal dose. Both deficiency and excess of coagulant lead to a decrease in its coagulant capacity [10,11]. The choice of coagulant as well as its dose depends, in turn, on the type of treated water/sewage, their concentration, and is carried out empirically.

The coagulation–flocculation and sedimentation processes are usually examined in natural systems [12–14], as well as in modeled systems, such as silica suspension [15,16]. The complexity of the coagulation–flocculation processes, the number of factors affecting their course, as well as a number of limitations regarding the possibilities of conducting laboratory experiments, prevent a thorough examination and elucidation of the processes and their kinetics. In such conditions, there is a need for new methods of studying these processes. Limitations in the area of laboratory experimentation can be overcome by computer simulation of the coagulation process. This method not only ensures full control over the process being studied, but it also offers nearly limitless opportunities for its modeling. Therefore, the purpose of this work was to use computer simulation to study the coagulation process. To study the effect of the degree of dispersion and the concentration of colloidal suspension on the kinetics of the coagulation process. As mentioned before, the efficiency of coagulation is determined, among others, by the type and concentration of impurities removed. Therefore, research on their effect on coagulation and its kinetics is justified. For example, it has been proven that the effectiveness of coagulation in removing organic impurities from water is directly proportional to their molecular weight. [17]. Research on coagulation–flocculation processes are most often done empirically. However, modeling this process not only helps to better understand the laws that govern it, but also has great practical significance. Coagulation kinetics modeling of water treatment plants can be used for process optimization and testing of control strategies to meet effluent quality requirements at a reasonable cost. In many countries, simulation software has become a standard tool for designers and

workers of modern wastewater treatment plants, and the findings of such studies and measurements are increasingly useful from a practical perspective [18–20].

Coagulation–flocculation processes were examined in this study with an original piece of computer software – ZB2. It simulates the coagulation–flocculation–sedimentation process in a system containing spherical particles of wastewater suspension and spherical coagulant particles. The results of simulation studies were tested by conventional kinetic equations for first and second-order reactions. The respective reaction rate constants and the effect of the wastewater suspension concentration on the coagulation–flocculation rate was determined. The effect of the dispersion degree and the suspension particle density on the coagulation process kinetics were examined.

2. Methods

2.1. Description of the simulation model

The ZB2 computer program was used in the study to simulate the coagulation–flocculation and sedimentation process in the wastewater suspension. The software was created based on long-term studies of coagulation and electrocoagulation processes conducted with natural and model wastewater.

The ZB2 simulation program is a stochastic-dynamic model; its operation is based on random variables and the system status changes with the passing of simulation time. The module which solves the motion equation for a specific number of matter points (particles) in a closed container is the core of the program. The ZB2 program simulates coagulation–flocculation–sedimentation of polydispersion sol; since there are type I and II spherical particles, which can differ by size, mass, initial velocity, the particles can simulate particles of coagulant and sol. The particles initial positions are generated randomly in accordance with uniform distribution in the container area. The particles move by Brownian motion. The program calculates the motion route for each particle separately, and the motion direction is chosen by the RANDOM function. The angle of reflection from a container wall is always equal to the angle of incidence. The initial velocity (V) is assigned randomly to each particle.

The program simulates the process of fast, perikinetic coagulation, in which each collision of a coagulant and sol particle results in the formation of an indissoluble bond; particles of the same type do not form a bond. If two particles of different velocities collide, they join and the direction and velocity of the resulting bunch (dimer) is the resultant vector. The sedimentation rate increases when the number of sol particles in a bunch increases. For the simulation of particle friction against a liquid, the floc velocity towards the surface is decreased by 0.1% per shift unit. When an aggregate reaches a predefined size, which is termed “coagulation threshold” (E), aggregates sediment and drop out of the system. The coagulation threshold determines how many sol particles sedimentation starts; it is determined so that there is a specific, predefined number of sol particles per coagulant particle.

The ratio of a coagulant particle mass to sol particle mass (m_c/m_s) depends on the coagulant and sol particle sizes and

it is calculated as $m = d \cdot V$; coagulant and sol particles are spheres, therefore $V = 4/3\pi r^3$, hence:

$$\frac{m_c}{m_s} = \frac{d_c \cdot 4/3\pi \cdot r_c^3}{d_s \cdot 4/3\pi \cdot r_s^3} \quad (1)$$

where d_c = coagulant density, d_s = sol density, r_c = coagulant radius, r_s = sol radius.

The program has the S = stop function, which measures the simulated process duration, and the number of “coagulated” particles in the sediment.

2.2. Input parameters of the simulation model

The following input data were taken sequentially in the simulation:

- N_c – coagulant particle number; in the study $N_c = 20, 40, 60, 80, 100, 120,$ and 140 .
- N_s – sol particle number; in the study $N_s = 200, 400, 600, 800, 1,200,$ and $1,400$.
- V_c – initial velocity of the coagulant particle; $V_c = 100 = \text{const}$.
- V_s – initial velocity of the sol particle; $V_s = 100 = \text{const}$.

Each individual particle was randomly assigned its initial speed, $V_c = V_s = 100$, this means that all particles were assigned a speed in the range of 1–100, and the program prevents any particle from having an initial speed equal to zero. After the collision of two particles which have different velocities results in the formation of a cluster (e.g. a dimer) whose direction and new velocity are resultants calculated and then converted into vectors.

- E – coagulation threshold; $E = 10 = \text{const}$.
- F – sedimentation coefficient; $F = 0.2 = \text{const}$.

The sedimentation coefficient– F is a systemic parameter specifying the range of “settling values” assumed by a cluster. Rate of sedimentation F takes into account that the velocity of a floc decreases by 30% when it bounces off the vessel bottom. To simulate particle-fluid friction, the velocity of a floc moving towards the surface was reduced by 0.1% per unit of displacement.

- r_c – coagulant particle radius; $r_c = 1 = \text{const}$.
- r_s – sol particle radius; $r_s = 1, 2, 3, 4, 5,$ and 6 .
- m_c/m_s – rate of coagulation particle mass to sol particle mass; $m_c/m_s = 1 = \text{const}$.

In most cases, such values of simulation input parameters were applied so that they corresponded to the wastewater reality or to the reality of the laboratory jar-test.

All units were simulation units; for example, time is the simulation second (s). The size of coagulant particles (r_c) and sol particles (r_s) was at the lower limit of colloidal particle size, and it could be expressed in simulated nanometers (nm). The initial particle velocity is expressed in simulated units mm s^{-1} that represent the quotient of the simulated distance and the simulated time. In this study, the motion of

particles was accelerated with a simulated stirrer used under laboratory conditions and in wastewater plants.

Time (t) was measured in five replicates and the arithmetic average was calculated after the lowest and the highest values were rejected. The standard deviation values were added to the respective graphs. The program had been positively verified based on the principles of the classical kinetic theory and dispersoid diffusion, and it complies with the logic and the general principles of colloidal system destabilization [19,21,22]. The verification of the program was done in a wide range of output parameters. For verification of the measurement database, there were applied classic, fundamental mathematical relationships resulting from the theory of Smoluchowski and Müller, empirical formulas, formulas constituting the conversion of the fundamental equation.

Table 1 shows the actual number of particles in the simulated system after time compared to the number of particles calculated on the basis of the classic Smoluchowski and Muller equations. The number of particles calculated theoretically from the Smoluchowski and Muller equations differed from the number of particles in the simulation system after the time t , generally with a few-percent deviation. The table shows only the sample results. In general, deviations Δ between theoretically calculated numbers and real values (for a wide range of output parameters) were in the range of 0 to 13.3%, which provides an accuracy of the simulated model.

3. Discussion and results

3.1. Determination of the order of a simulated wastewater suspension coagulation process

The order of the simulated coagulation process was determined graphically by conversion of the I and II order kinetic reaction:

$$\frac{dN_s}{dt} = -k_I \cdot N_s \quad \frac{dN_s}{dt} = -k_{II} \cdot N_s^2 \quad (2)$$

$$t = \frac{1}{k_I} \cdot \ln \frac{N_{s0}}{N_s} \quad t = \frac{1}{k_{II}} \cdot \left(\frac{1}{N_s} - \frac{1}{N_{s0}} \right) \quad (3)$$

where N_{s0} – primary number of the sol particles k_I and k_{II} – constant ratios of the first and second-order respectively.

The graphs show linear relationships of $t = f(\ln 1/N_s)$ (Figs. 1a and c) and $t = f(1/N_s)$ (Figs. 1b and d) for the simulation systems, in which the initial sol concentration is $N_s = 400$ (Figs. 1a and b) and $N_s = 1,200$ (Figs. 1c and d). The sol particle radius is equal to the coagulant particle radius: $r_s = r_c = 1$. The ratio of coagulant particle mass to sol particle mass is constant: $m_c/m_s = 1$. The initial velocity of the sol and the coagulant particles is the same: $V_s = V_c = 100$. The determination coefficients R^2 for the four linear regressions presented here lay within the high-value range of 0.93 to 0.98; however, a clearly more favorable kinetic equation for the sol coagulation rate was not identified for the pairs of general relationships $t = f(\ln 1/N_s)$ and $t = f(1/N_s)$.

Table 1

Actual number of particles in a simulated system compared to a number of particles calculated based on the Smoluchowski and Muller equations

Actual number of particles in the simulated system	Number of particles calculated from Smoluchowski equation	Deviation parameter Δ (%)	Average deviation parameter Δ (%)	Number of particles calculated from Muller equation	Deviation parameter Δ (%)	Average deviation parameter Δ (%)
$N_c = 100; N_s = 1,000; F = 0.2; I = 1; E = 10; R_c = 2; R_s = 2$						
990	976	1.4	3.9	965	2.5	5.8
880	926	5.2		911	3.5	
770	844	9.6		825	7.1	
660	638	3.3		612	7.3	
550	550	0		524	4.7	
440	423	3.9		398	9.5	
$N_c = 50; N_s = 1,000; F = 0.2; I = 1; E = 15; R_c = 2; R_s = 2$						
970	932	3.9	2.7	926	4.5	3.9
890	894	0.4		887	0.3	
810	809	0.1		799	1.2	
730	705	3.4		693	4.9	
650	622	4.3		609	6.2	
570	546	4.2		533	6.5	

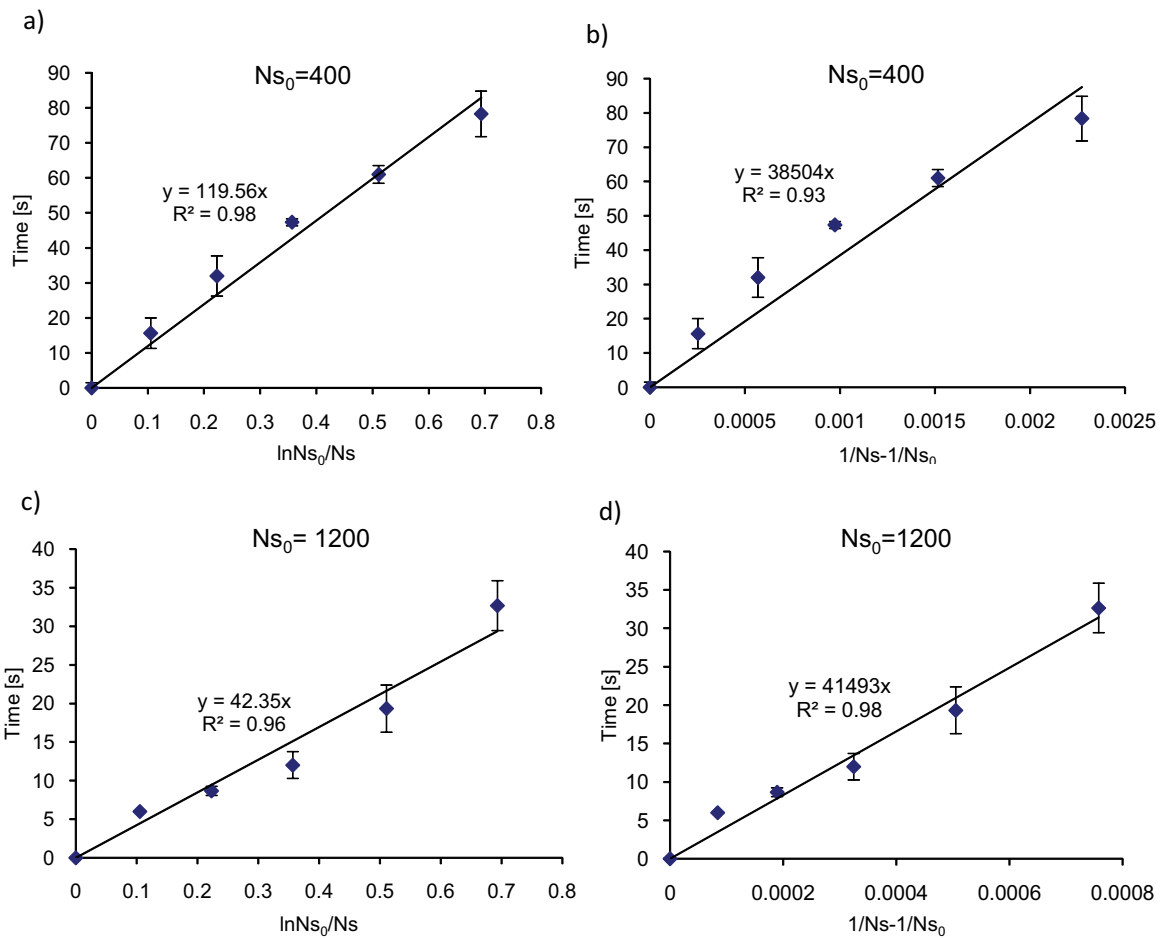


Fig. 1. Example relationships $t = f(\ln(1/N_s))$ (a and c) and $t = f(1/N_s)$ (b and d) for a simulated coagulation process at sol concentrations of $N_s = 400$ and $1,200$.

Tables 2 and 3 lists all the values of R^2 determined for the mathematical models of $t = f(\ln 1/N_s)$ and $t = f(1/N_s)$. The determination coefficients R^2 applied to different simulated coagulation systems. Table 2 lists R^2 values for simulation systems in which the sol concentration increased from $N_s = 200$ to $N_s = 1400$; the sol and coagulant particles size was the same: $r_s = r_c = 1$. The sol and coagulant particle velocity was $V_s = V_c = 100$. The sol particle density remained constant, the ratio of the coagulant particle mass to sol particle mass was constant: $m_c/m_s = 1$. Table 3 lists R^2 values for the simulated coagulation process systems, with the sol particle initial velocity of $N_s = 400$ and $N_s = 800$, the sol particle radius in these systems was changed from $r_s = 1$ to $r_s = 6$, while the coagulant particle radius remained constant at $r_c = 1$. The ratio of the coagulant particle mass to sol particle mass remained constant $m_c/m_s = 1$ with an increasing ratio of the sol particle radius to coagulant particle radius, that is, the sol density decreased with increasing size of its particles. The sol and coagulant particle motion velocity were constant $V_s = V_c = 100$. Although the study of destabilization kinetics of a simulated suspension showed that the relationships $t = f(\ln 1/N_s)$ and $t = f(1/N_s)$ are linear with a high determination coefficient (from $R^2 = 0.90$ to 0.99), they did not identify a clearly more favorable kinetic equation to describe the simulated sol coagulation rate. The average R^2 for $t = f(\ln 1/N_s)$, (for all the simulation systems under test), was 0.97 and it was slightly higher than R^2 for $t = f(1/N_s)$ with an average of 0.95 . Therefore, the coagulation process rate within the range described in the simulated system was consistent with both the first and second-order rate equations. The practical side of coagulation often leads to similar doubts. The linearity of the relationships identified in the simulated system has been confirmed in a number of papers describing the results of laboratory experiments and those verifying the consistency of the Smoluchowski theory with experimental data [23–25].

3.2. Effect of sol concentration on the colloidal suspension coagulation-flocculation rate

Fig. 2 shows a comparison of the reaction rate constants (k) in the simulated coagulation systems in which the initial

sol concentration changed from $N_0 = 200$ to $N_0 = 1400$, the sol particle and coagulant particle radius was constant: $r_s = r_c = 1$, the density was $d_s = d_c$, $m_c/m_s = 1$ and the motion velocity was $V_s = V_c = 100$.

As expected, the reaction rate (k) increased each time the sol concentration grew. The maximum $k = 3.85 \times 10^{-2}$ at a sol concentration of $N_0 = 1400$ was more than five times higher than $k = 7.28 \times 10^{-3}$ calculated for the sol concentration of $N_0 = 200$. Therefore, a seven-fold increase in the sol concentration resulted in a five-fold increase in the reaction rate. A theory of fast coagulation for mono-dispersion systems was developed by Marian Smoluchowski (1916); the theory assumes that colloidal particles are spherical and every collision is effective in forming an aggregate, so that the collision efficiency = 1. Two spherical particles, undergo an aggregation when they approach one another to a distance smaller than the attraction zone radius, thus the aggregation occurs practically on their direct contact. The number of the particle collisions is defined only by translational Brownian motion. According to Smoluchowski [26], the probability (W) of particle collision is higher along with a larger particle shift caused by Brownian motion per time unit and a larger attraction zone radius (A) for equal-radius particles:

$$W = 4\pi AD \tag{4}$$

where: A denotes the attraction zone radius, whereas D is a diffusion coefficient, which is a measure of shift in Brownian motion.

According to Fick's law for concentrated solutions, in which the diffusion coefficient (D) depends on the concentration, the following equation can be formulated, which binds so called "diffusion current" $\delta c/\delta t$ and the concentration gradient $\delta c/\delta x$:

$$\frac{\delta c}{\delta t} = \frac{\delta}{\delta x} \left[D \left(\frac{\delta c}{\delta x} \right) \right] \tag{5}$$

where: x denotes a generalised coordinate.

Eq. (3) shows that the diffusion current $\delta c/\delta t$ is directly proportionate to the diffusion coefficient (D). In theory, a concentration increase should be accompanied by an increase

Table 2
The R^2 values for $t = f(\ln 1/N_s)$ and $t = f(1/N_s)$ in simulation systems at increasing sol concentrations N_s

R^2 for $\ln 1/N_s$		R^2 for $1/N_s$	
N_s	R^2 $r_s = r_c = 1$	N_s	R^2 $r_s = r_c = 1$
200	0.96	200	0.90
400	0.98	400	0.92
600	0.99	600	0.97
800	0.96	800	0.92
1,000	0.93	1,000	0.97
1,200	0.96	1,200	0.98
1,400	0.95	1,400	0.90
	Mean $R^2 = 0.96$		Mean $R^2 = 0.94$

Table 3
The R^2 values for $t = f(\ln 1/N_s)$ and $t = f(1/N_s)$ in simulation systems at sol concentrations of $N_s = 400$ and 800 and increasing sol particle radius

r_s	R^2 for $\ln 1/N_s$		r_s	R^2 for $1/N_s$	
	R^2	R^2		R^2	R^2
	$N_s = 400$	$N_s = 800$		$N_s = 400$	$N_s = 800$
1	0.98	0.96	1	0.92	0.92
2	0.97	0.95	2	0.99	0.92
3	0.93	0.97	3	0.94	0.94
4	0.94	0.98	4	0.96	0.95
5	0.98	0.99	5	0.95	0.97
6	0.97	0.99	6	0.93	0.98
	Mean $R^2 = 0.97$		Mean $R^2 = 0.95$		

in the diffusion coefficient (D) and the related probability of colloidal particle collisions.

3.3. Effect of the sol dispersion degree on the colloidal system destabilization time

The Fig. 3 shows a comparison of the reaction rate constants (k) in the simulation coagulation systems in which the sol particle radius changed from $r_s = 1$ to $r_s = 6$, the coagulant particle radius was constant: $r_c = 1$. The effect of the dispersion degree on the reaction rate constants was examined in the system of initial concentration of $N_0 = 400$ (series I) and in the system of twice higher concentration $N_0 = 800$ (series II). The sol and coagulant particle motion velocity was constant $V_s = V_c = 100$, whereas the sol particle density decreased with increasing particle radius with $m/m_s = 1$.

Each increase in the sol particle radius (the coagulant particle radius $r_c = 1 = \text{const}$) was accompanied by an increase in the reaction rate (k), regardless of the sol concentration. And so the maximum rate constant of $k = 8.62 \times 10^{-2}$ at the sol concentration of $N_s = 800$ was nearly seven times higher than $k = 1.28 \times 10^{-2}$ calculated for the sol particle radius of $r_s = 1$. The six-fold increase in the sol particle radius resulted in a nearly seven-fold increase in the reaction rate constant.

Moreover, an effect of the sol particle size on the reaction rate constants in lower concentration systems was found to be greater. For a simulation system in which the sol concentration was twice lower ($N_s = 400$), a six-fold radius increase resulted in a nearly eight-fold increase in the reaction rate constant. A similar tendency was observed in other cases $N_s = 200, 600, 1000, 1200, 1400$. Each time the sol particle radius increased, the reaction rate (k) increased, regardless of the sol concentration.

An increase in the sol particle radius made the mono-dispersion system turn into a polydispersion system; along with the coagulant particles of the constant radius $r_c = 1$, there were sol particles of the radius of $r_s = 2, 3, 4, 5, 6$. According to the Smoluchowski theory, extended by Muller to cover polydispersion systems, probability “ W_1 ” of a collision of two particles of different sizes is greater than the respective probability in the case of equal-radius particles:

$$W_1 = 2\pi(r_s + r_c)(D_s + D_c) \tag{6}$$

The active attraction radius is the sum of the large and the small particle. Therefore, an increase in the sol particle radius was followed by an increase in the attraction zone

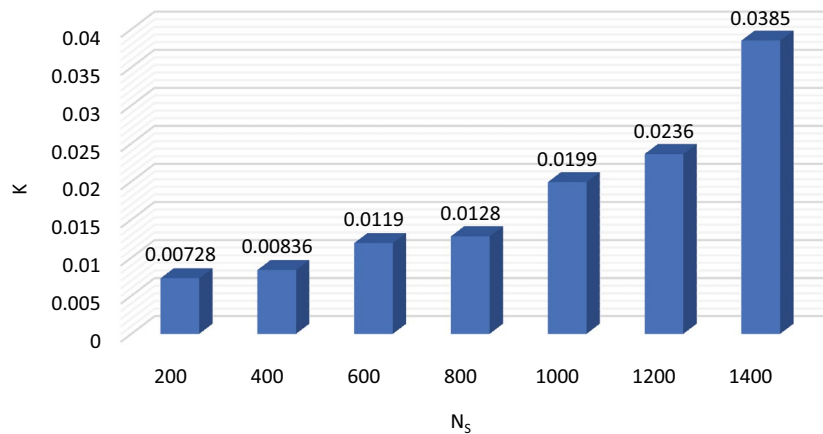


Fig. 2. Effect of sol concentration (N_s) on the coagulation rates.

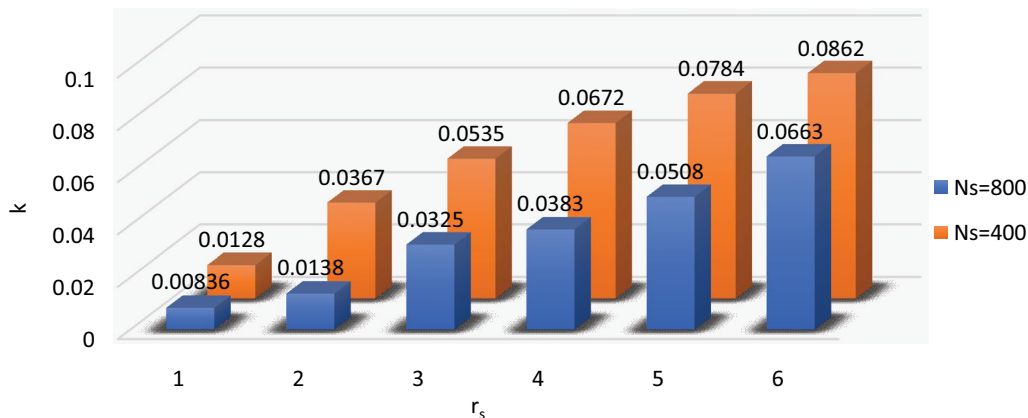


Fig. 3. Effect of sol particle size (r_s) on coagulation rate constants; series I sol concentration $N_s = 400$, series II sol concentration $N_0 = 800$.

radius, that is, an increase in the probability of particle collisions and aggregation, which resulted in accelerated coagulation.

3.4. Effect of sol particle size and sol concentration on initial coagulation and reaction half-life

An important phase of the coagulation–flocculation process is what is referred to as initial coagulation, during which the coagulation process is not accompanied by visible changes (colour, cloudiness, etc.). Initial coagulation often affects the entire coagulation process and it can ultimately have a deciding effect on the effectiveness of the entire coagulation process. Another important factor for the coagulation process kinetics is the reaction half-life, during which the number of all the colloidal particles in the system is reduced by half compared to the initial number. Fig. 4 shows the effect of the sol particle size on the time needed for destabilising 10% of the system (Fig. 4a) and on the time needed for destabilising 50% of the system (Fig. 4b). The simulation was conducted for two different initial sol concentrations $N_0 = 400$ (curve I) and for a twice higher concentration of $N_0 = 800$ (curve II). The maximum fitting of the results $R^2 \geq 94$ was achieved for $y = ax^b$. The

respective equations and R^2 were placed on graphs. An analysis of the curves and the equations that describe them shows that the terms “ b ” in the equations $y = ax^b$ lay within a relatively narrow range of -1.07 to -1.18 , which may indicate that they are independent of the degree of the colloidal system destabilization. Therefore, the “ a ” term is responsible for the variability of the curves. Each time the sol particle radius increased, the time needed for destabilization of 10% or 50% of the system decreased. On the other hand, the effect of the sol concentration on the time of the colloidal system destabilization time decreased with increasing sol particle size. For example, when the sol particle radius $r_s = 1$, the time difference needed for destabilization of 50% of the system at the initial sol concentration of $N_0 = 400$ and $N_0 = 800$ was 30 simulation seconds. On the other hand, an increase in the sol radius to $r_s = 6$ reduced the difference to 1.3 simulation seconds.

A comparison of the term “ a ” in equations $y = ax^b$ shows a more distinct effect of the sol concentration and its particle size for 50% destabilization, where the respective terms $a = 87.95$ and $a = 43.549$ are nearly five times greater than $a = 19.649$ and $a = 9.654$ in the equations for 10% destabilization. This may indicate that the sol particle size has a small effect on the initial coagulation rate.

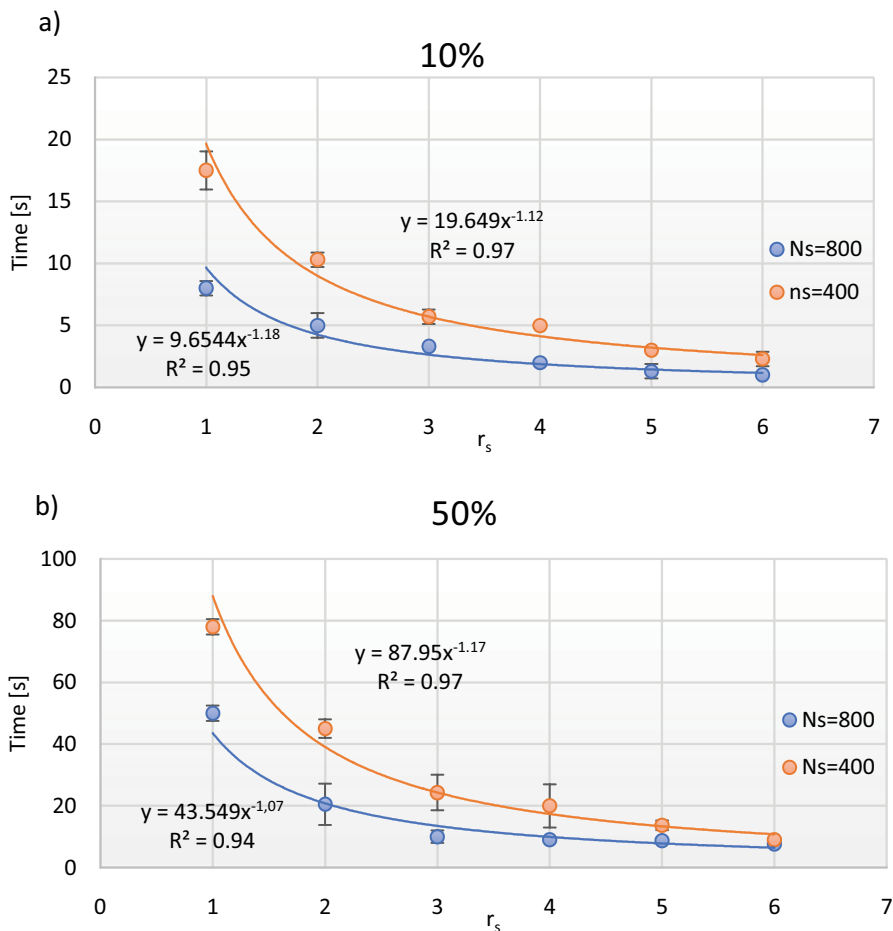


Fig. 4. The time necessary for the destabilization of (a) 10% of the system particles and (b) 50% of the system particles depending on the dispersion degree and sol concentration.

4. Summary and conclusions

The study of the effect of the degree of dispersion and sol concentration on the simulated sol destabilization kinetics showed the linearity of the relationships $1/N_{(t)}$ and $\ln 1/N_{(t)}$ supported by a high value of the determination coefficient R^2 . The coagulation process rate within the range described in this paper was consistent with both the first and second-order rate equation. An increase in the sol concentration brought about an increase in the coagulation process rate expressed as an increase in the reaction rate constant. A seven-fold increase in the sol concentration brought about a five-fold increase in the reaction rate. An increase in the sol concentration increased the probability of colloidal particle collisions and, in consequence, increased the reaction rate.

The simulated coagulation rate depended on the colloidal suspension dispersion degree and increased along with an increasing ratio of sol particles radius to the coagulant particles radius. The simultaneous presence of larger and smaller particles accelerated the coagulation of any system. A six-fold increase in the sol particle radius $r_s/r_c = 6/1$ resulted in a 6.9-fold increase in the reaction rate constant compared to the coagulation system in which $r_s/r_c = 1/1$. An effect of the sol particle size on the reaction rate was even greater for the sol of a two-fold lower concentration: a six-fold increase in the radius resulted in 7.9-fold increase in the rate constant for the simulated reaction of coagulation–flocculation of the colloidal suspension. According to Müller's theory, the probability of a collision of two particles of different sizes is greater than the probability of a collision of equal radius particles. The attraction zone radius for polydispersion sol, consisting of two types of particles of different radii is the sum of the radii. Therefore, an increase in the sol particle radius was followed by an increase in the attraction zone radius, that is, an increase in the probability of particle collisions and aggregation, which resulted in accelerated coagulation.

The sol particle size and suspension concentration (within the tested range) had little effect on the initial coagulation rate, whereas a considerable effect of the sol particle size and its concentration was observed for the coagulation half-life.

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