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COMPUTER SIMULATION OF FLOCCULATION AND CHEMICAL COAGULATION

SYMULACJA KOMPUTEROWA PROCESU FLOKULACJI I KOAGULACJI CHEMICZNEJ

Abstract: In the present study, a computer program was employed to simulate the coagulation of suspended solids. The paper provides a description of the developed simulation program. The reaction order of the coagulation process was determined, and the effect of the initial velocity of sol particles and the size of sol and coagulant particles on the rate of coagulation was investigated. The tested program was found to comply with the classical theories of particle motion and colloidal system destabilization. The rate of the simulated coagulation process satisfied second-order kinetic equations and the Smoluchowski equation. As expected, a simulated increase in the initial velocity of sol particles increased the rate of coagulation. An increase in the sol particle diameter had a more significant effect on the rate of coagulation than an increase in the coagulant particle diameter.

Keywords: coagulation, flocculation, simulation, sol

Although the technologies of chemical and biological-chemical wastewater treatment are constantly being improved, coagulation remains the most popular and widely applied method. The complex coagulation-flocculation process can be classified as orthokinetic or perikinetic. In orthokinetic coagulation, the particles collide due to the effect of external factors. The process may be accelerated by stirring which increases the probability of collisions between single colloidal particles and agglomerates. The final result of orthokinetic coagulation is dependent upon the amount of mechanical energy dispersed per unit volume. An excessive amount of energy prevents colloid flocculation [1], and the force of gravity may inhibit the gelation of suspended solids [2]. In perikinetic coagulation, the particles move by random Brownian motion and collide. Perikinetic coagulation takes place, among others, in pre-sedimentation and

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septic tanks at wastewater treatment plants. Since colloidal particles suspended in wastewater have low kinetic energy, destabilization and colloid precipitation occur at a slow rate.

Due to its complexity, the coagulation process continues to receive the attention of researchers and practitioners, and it is studied from both a fundamental (the mechanism and kinetics of particle flocculation) [3–6] and a utilitarian perspective [7–8]. Coagulation, aggregation, flocculation and sedimentation processes are usually investigated in natural systems, such as wastewater [9, 10], model systems, including silica suspensions [11], as well as computer-simulated systems [12–14]. Computer-assisted simulations offer unlimited experimental options, supporting the description of molecular collision models, the mechanism of latent, slow and rapid coagulation, as well as the conditions and the kinetic parameters of those processes [15–19]. The results of computer-aided simulations support the development of fundamental databases, and the resulting conclusions and suggestions [20] render them an interesting alternative to applied research.

Contemporary research often relies on Monte Carlo simulation methods. This approach is based on the theory of probability and statistical mechanics, and it is widely applied to calculate the fractal dimensions of aggregates, investigate their structure, and to study the mechanism of aggregation, coagulation and flocculation processes [21–25].

In the present study, a computer program (ZB2) was employed to simulate the coagulation of suspended solids. The kinetics of chemical coagulation and the reaction order of the coagulation process were determined. The effect of the initial velocity of sol particles and the size of sol and coagulant particles on the rate of coagulation was also investigated.

Methods

The ZB2 program was written in Pascal. The program simulates the coagulation, flocculation and sedimentation of spherical sol particles with the use of spherical coagulant particles [26]. The applied simulation model is a stochastic and a dynamic model based on random variables, and its state changes over simulation time. The simulation program features a module solving the equation of motion of a given number of points (particles) in a closed vessel. The initial particle location values are randomly generated in line with a homogenous system in the vessel area. The direction of particle movement and their initial location are randomly drawn using the RANDOM command. The angle at which a particle hits the wall is always equal to the angle of incidence. The velocity of a cluster that hits the bottom decreases by 30 %. The following input data were adopted:

- A – number of coagulant particles: $A = \text{const} = 100$;
- B – number of sol particles: $B = \text{const} = 1000$;
- C – initial velocity of a coagulant particle: $C = 5, 10, 15, 20, 25, 30, 35$ and 40 ;
- D – initial velocity of a sol particle: $D = 2C$, ie, $10, 20, 30, 40, 50, 60, 70, 80$ and $D = 5C$, ie, $25, 50, 75, 100, 125, 150, 175$ and 200 ;

- E – “coagulation threshold”, ie a parameter indicating the number of sol particles which initiate the sedimentation of a cluster/floc containing one coagulant particle: $E = \text{const} = 10$;
- F – “sedimentation coefficient”: $F = \text{const} = 0.2$;
- G – simulated average diameter of a coagulant particle. Changes in G are not displayed on the screen, but they become visible as the distance between the particles in the formed floc increases. The smaller the diameter of the coagulant particle, the lower the probability of collision with a sol particle: $G = 1, 2, 3$ and 4 ;
- H – simulated average diameter of a sol particle: $H = 1, 2, 3$ and 4 ;
- I – simulated ratio of the mass of a coagulant particle to the mass of a sol particle determined by the values of G and H .

The program was equipped with the S = stop function (timer) measuring the time of the simulated process as well as a meter counting the number of “coagulated” particles in the sediment because the program counts particles with the velocity of $C = 0$.

All tests were performed in seven replications. Two maximum values and two minimum values were discarded to compute the arithmetic mean based on three measurements.

Results and discussion

In line with the adopted methodology, the number of deposited coagulant particles A and the number of sol particles B (waste) was counted every time after stimulated time t [simulated second]. Reaction order was determined graphically through the conversion (linearization) of generally applied kinetic equations of first-order (a) and second-order (b) reactions, respectively:

$$\text{a) } t = f \{2,303 \ln [1100/(A + B)]\},$$

$$\text{b) } t = f [1/(A + B) - 1/1100].$$

The number 1100 appearing in equations a) and b) is the initial, ie at $t = 0$, total number of coagulant particles A and sol particles B in the system:

$$1100 = A(100) + B(1000)$$

Tables 1 and 2 demonstrate the effect of changes in the initial velocity of each coagulant particle C , accompanied by the proportional values of the initial velocity of each sol particle D , on the rate of the coagulation process.

$$D = 2 \cdot C - \text{Table 1, } D = 5 \cdot C - \text{Table 2}$$

In practice, changes in the initial velocity of any particle result from alterations in temperature or stirring intensity, since both parameters always lead to changes in the studied object’s kinetic energy.

Table 1

The values of first-order and second-order reaction rate constants and the values of determination coefficient R^2 for C and D pairs from 5 and 10 to 40 and 80

C, D, E, G, H, I	R^2 for I order	$k_I \cdot 10^{-2}$	R^2 for II order	$k_{II} \cdot 10^{-5}$
5; 10; 10; 2; 2; 1	0.899	1.58	0.971	0.916
10; 20; 10; 2; 2; 1	0.941	1.98	0.991	1.16
15; 30; 10; 2; 2; 1	0.921	2.13	0.980	1.24
20; 40; 10; 2; 2; 1	0.946	2.29	0.988	1.34
25; 50; 10; 2; 2; 1	0.970	2.94	0.981	1.73
30; 60; 10; 2; 2; 1	0.978	3.51	0.984	2.07
35; 70; 10; 2; 2; 1	0.957	3.39	0.988	1.99
40; 80; 10; 2; 2; 1	0.968	3.89	0.981	2.29

Table 1 presents selected k_I , k_{II} and R^2 values for C and D pairs from 5 and 10 to 40 and 80. As anticipated, an increase in the particles' initial velocity was accompanied by an increase in the rate of the investigated coagulation process, expressed by the rate constants of both first-order (k_I) and second-order reactions (k_{II}). The values of the corresponding coefficients of determination R^2 for the second-order model were always higher than for the first-order model. The use of a second-order model in the examined simulation produced an average $R^2 = 0.983$, which was higher than the average $R^2 = 0.948$ reported in the first-order model.

Table 2

The values of first-order and second-order reaction rate constants and the values of determination coefficient R^2 for C and D pairs from 5 and 25 to 40 and 200

C, D, E, G, H, I	R^2 for I order	$k_I \cdot 10^{-2}$	R^2 for II order	$k_{II} \cdot 10^{-5}$
5; 25; 10; 2; 2; 1	0.934	1.86	0.985	1.08
10; 50; 10; 2; 2; 1	0.951	3.17	0.987	1.85
15; 75; 10; 2; 2; 1	0.976	3.72	0.950	2.21
20; 100; 10; 2; 2; 1	0.938	4.66	0.977	2.73
25; 125; 10; 2; 2; 1	0.913	5.58	0.965	3.25
30; 150; 10; 2; 2; 1	0.886	6.98	0.935	4.08
35; 175; 10; 2; 2; 1	0.923	7.61	0.949	4.47
40; 200; 10; 2; 2; 1	0.927	8.16	0.929	4.81

Table 2 illustrates selected k_I , k_{II} and R^2 values for C and D pairs from 5 and 25 to 40 and 200. Similarly to the data shown in Table 1, the values of the corresponding coefficients of determination R^2 for the second-order model were higher in comparison with the first-order model. The use of a second-order model in the studied process produced an average $R^2 = 0.960$, which was also higher than the average $R^2 = 0.932$ for the first-order model. The results indicate that the coagulation process was a second-order reaction. This suggests that the applied ZB2 system is fully consistent with Smoluchowski's theory of coagulation kinetics [27], and the coagulated system has the

features of a monodispersive sol. In view of the observed results, $G = H$, therefore, the average diameter of a coagulant particle was identical to the diameter of a sol particle.

The correlation between the coagulation rate (k_{II}) and the initial velocity of sol particles D is illustrated in Figs. 1a and 1b. It was assumed that the kinetic energy (initial velocity) of a single coagulant particle should be at least twice lower than the kinetic energy of a single sol particle because the aim of every coagulant particle is to “collect” 10 sol particles, and not the other way around. For this reason, in Fig. 1a, the initial velocity of coagulant particles, determined in the range of $D = 10$ –80, was set at half the initial velocity of sol particles ($C = 5$ –40), whereas the data shown in Fig. 1b, covering a more extensive range of $D = 25$ –200, always required $D = 5C$ to support the examination of a range identical to that in Fig. 1a ($C = 5$ –40). Therefore, Figs. 1a and 1b demonstrate the effect of the initial velocity of two types of sol particles on the coagulation rate with the use of an identical coagulant. The resulting database effectively illustrates the simulation of the coagulation of different sols using the same coagulant. The simulated variation in the initial velocity of a sol particle, where particle diameter ($G = H = 2$) and the density of sol and coagulant particles ($I = 1$) remained constant, implies that the simulated coagulation took place after the preliminary heating of sol from the temperature indicated in Fig. 1a to that in Fig. 1b, or after the preliminary, intense stirring of sol particles in Fig. 1a to achieve the velocity shown in Fig. 1b. Coagulant particles were introduced to the system after the heating or stirring of the “waste”, and they were subjected to the analyses shown in Fig. 1b.

In the range of $D = 25$ –80, shared by both figure drawings, preliminary heating (or stirring) had an insignificant effect on the coagulation rate (k_{II}), although every simulated increment in sol particles’ initial velocity increased the coagulation rate within the entire measurement range. According to the data in Fig. 1b, the maximum coagulation rate is $k_{II} = 4.81 \cdot 10^{-5}$, while in Fig. 1a, the maximum coagulation rate is $k_{II} = 2.29 \cdot 10^{-5}$ at the same initial velocity of coagulant particles. The above implies that $D = 200/D = 80$, therefore, a 2.5-fold increase in sol particles’ initial velocity produces only $4.81/2.29 = 2.1$ -fold increase in the studied sol’s coagulation rate.

According to Fig. 1a, the value of k_{II} calculated from a regression equation reached $k_{II}(10) = 0.8981 \cdot 10^{-5}$ for $D = 10$ and $k_{II}(80) = 2.2841 \cdot 10^{-5}$ for $D = 80$. This

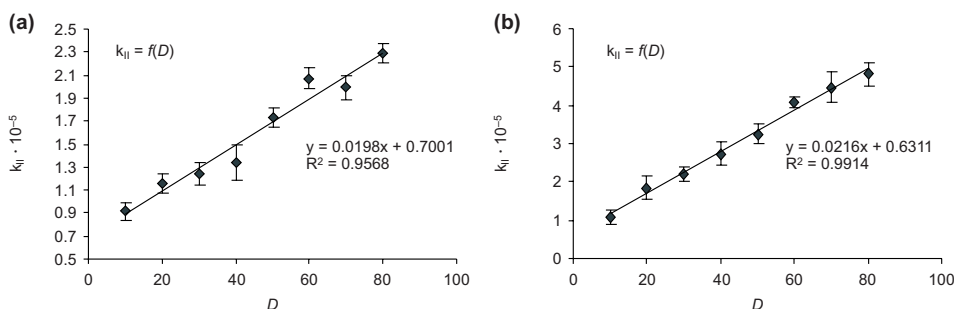


Fig. 1. The correlation between the coagulation rate and the initial velocity of sol particles (D) at a two-fold lower velocity of coagulant particles C , $D = 2C$ (a), at a five-fold lower velocity of coagulant particles C , $D = 5C$ (b)

demonstrates that an 8-fold increase in sol particles' initial velocity resulted in $2.2841/0.8981 =$ a mere 2.5-fold increase in the coagulation rate. Within the range shown in Fig. 1b, the value of k_{II} calculated from a regression equation reached $k_{II}(25) = 1.1711 \cdot 10^{-5}$ and $k_{II}(200) = 4.9511 \cdot 10^{-5}$. As above, an 8-fold increase in sol particles' initial velocity produced only $4.9511/1.1711 = 4.3$ -fold increase in the coagulation rate. The observed results support the following conclusion: " $D = 5C/D = = 2C =$ a 2.5-fold increase in sol particles' initial velocity produces only $4.3/2.5 =$ an estimated 1.7-fold increase in the rate of the simulated coagulation process". The above conclusion has a number of practical implications that can be laconically expressed as follows: before coagulation, ie before introducing the coagulant to the waste, the waste should not be **excessively** heated or stirred because the cost of those operations will not be compensated by the rate or the effectiveness of the waste coagulation (purification) process.

The effect of sol particles' diameter (H from 1 to 4) on the coagulation rate (k_{II}) at four values of G , ie $G = 1, 2, 3$ and 4 , is presented in Fig. 2. The ratio of a coagulant particle's mass to a sol particle's mass I was investigated on the assumption that coagulant and sol particles have identical density, therefore it was calculated each time as G^3/H^3 . The resulting graph comprises four \pm parallel, increasing linear functions, which is consistent with expectations because an increase in particle diameter maximizes the probability of an active collision. According to Arrhenius [28], the rate of any chemical reaction, including coagulation, is directly proportional to the number of active collisions in a unit of time. The simulated reaction (coagulation) shows that within the analyzed range, an increment in the value of H by one unit increases the reaction rate (k_{II}) by approximately $0.6 \cdot 10^{-5}$ (refer to the slopes of the respective straight lines in Fig. 2). The parallel lines in Fig. 2 remain separated by a fixed distance of approximately $0.3 \cdot 10^{-5}$ (k_{II}). Therefore, it can be postulated that an increment in the value of G by one unit increases the reaction rate by 20 %. In the examined combinations of G and H , the coagulation rate at $D = 2C$ was more affected by an

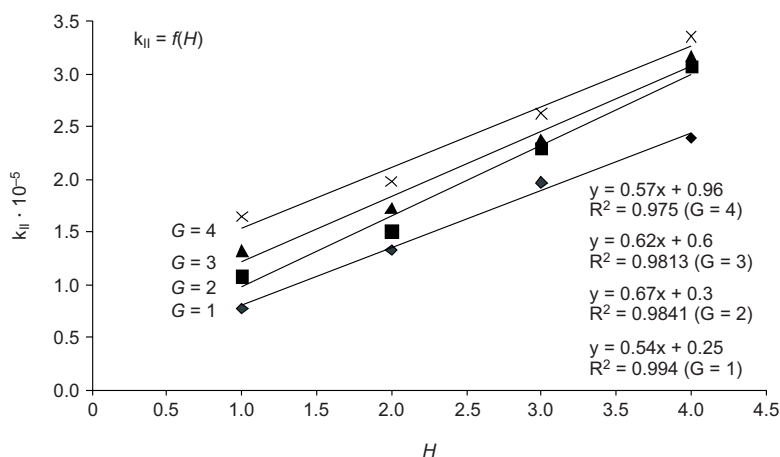


Fig. 2. The correlation between the coagulation rate and particle diameter at $D = 2C$

increase in the diameter of a sol particle than a coagulant particle. This fact is a logical consequence of the imposed proportions between the number of coagulant particles and sol particles at $A/B = 100/1000 = 0.1$. An increase in the diameter of sol particles marked by a 10-fold excess in the simulated coagulation system is more likely to increase the probability of an active collision with a coagulant particle than an increase in the diameter of coagulant particles remaining in a 10-fold minority.

Figure 3 illustrates the effect of sol particles' diameter (H from 1 to 4) on the coagulation rate (k_{II}) at two values of G , ie $G = 1$ and $G = 3$. Similarly to Fig. 2, the ratio of a coagulant particle's mass to a sol particle's mass I was investigated on the assumption that coagulant and sol particles have identical density, therefore, it was calculated as G^3/H^3 . As anticipated, the resulting graph comprises two parallel, increasing linear functions because an increase in particle diameter maximizes the probability of an active collision. The course of the simulated reaction (coagulation) indicates that within the studied range, an increment in the value of H by one unit increased the reaction rate (k_{II}) by approximately $0.62 \cdot 10^{-5}$ – as calculated from the regression equation for $G = 3$. This value closely approximates the results shown in Fig. 2. The parallel lines in Fig. 3 remain separated by a fixed distance of approximately $0.42 \cdot 10^{-5}$, which is nearly 1.5-fold greater than the distance indicated in Fig. 2. The absolute reaction rate values were higher by around 30–40 %, which does not correspond to the higher D values, from $D = 2C$ (Fig. 2) to $D = 5C$ (Fig. 3).

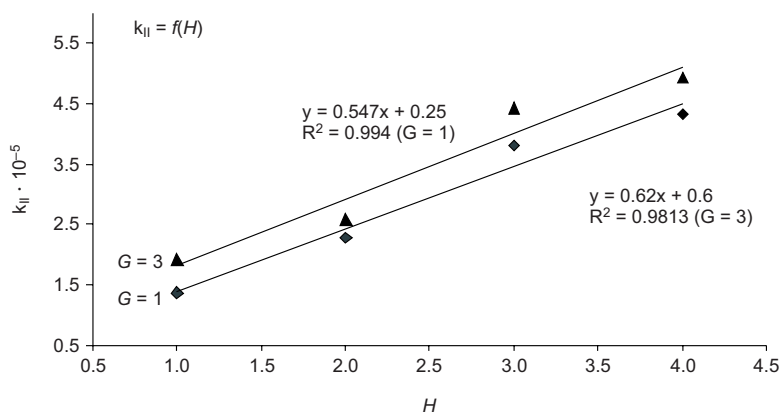


Fig. 3. The correlation between the coagulation rate and particle diameter at $D = 5C$

According to the kinetic theories postulated by Smoluchowski, Muller and others [27–29], the radius of a particle involved in the coagulation process affects the rate and the effectiveness of coagulation. Based on the work of Arrhenius [28] investigating the frequency of active collisions = reaction rate, eg k_{II} , the number of active collisions for second-order reactions is determined by particle radii as follows:

$$k_{II} \propto (G + H)^2$$

The above implies that the reaction rate is directly proportional to the square of total radii (diameters) of reagent particles. The results of this study do not “fit” the above

dependency. The discrepancies in the results of experiments investigating the kinetics of standard chemical reactions and laboratory experiments analyzing the coagulation kinetics of hydrosols have led to the creation and the popularization of the above coagulation kinetics theories (including Smoluchowski's theory). In different mathematical models, eg expressing the probability P that one particle will collide with another particle:

$$P = 4 \cdot \pi \cdot A \cdot D_r$$

where: A – radius of particle attraction, and D_r – coefficient of diffusion, the value of diffusion coefficient D_r is determined by the dimensions of coagulating particles.

The Smoluchowski formula and its modified version:

$$P = 4 \cdot \pi \cdot A \cdot D_r \cdot \xi$$

where ξ – fraction of effective collisions determined by coagulant concentrations, are used to determine the probability of particle collisions in both slow and rapid perikinetic coagulation of monodispersive sols. The methodological constraints of the discussed simulation prevented rapid or slow orthokinetic coagulation in the studied environment.

Summary and conclusions

This study investigated the effect of changes in the initial velocity of every coagulant particle C , combined with the proportional value of initial velocity of each sol particle D , because in practice, changes in the initial velocity of any particle result from alterations in temperature or stirring intensity, and both parameters always lead to changes in the studied object's kinetic energy.

The values of first-order and second-order reaction rate constants, k_I and k_{II} , and the respective values of determination coefficients R^2 indicate that the values of determination coefficients R^2 for the second-order reaction model were always higher than those noted in the first-order reaction model. The use of a second-order reaction model in the analyzed simulation was therefore correct from both the theoretical and the practical perspective. The ZB2 model complies with the theory of coagulation kinetics proposed by Smoluchowski, and the studied coagulation system has the features of a monodispersive sol.

The simulated variations in the initial velocity of a sol particle, where particle diameter ($G = H = 2$), sol and coagulant density remained constant ($I = 1$), show that the simulated process takes place after the preliminary heating or intense stirring of sol. Preliminary heating (or stirring) had an insignificant effect on the coagulation rate, although the anticipated stimulated increment in sol particles' initial velocity increased the coagulation rate within the entire measurement range. A 2.5-fold increase in sol particles' initial velocity resulted in only $4.81/2.29 = 2.1$ -fold increase in the coagulation rate.

The discussed experiment also investigated the effect of sol particles' diameter on the coagulation rate. The authors concluded that the rate of any chemical reaction, including

coagulation, is directly proportional to the number of active events. In the simulated process (coagulation), an increase in sol particles' diameter by a simulated unit accelerated the process by only 20 %. An increase in the diameter of sol particles was more likely to increase the rate of coagulation than an increase in the diameter of coagulant particles. The above was a logical consequence of the imposed proportions between the number of coagulant particles and sol particles. The increase in the coagulation rate resulting from a simulated increase in the size of sol particles proved to be smaller than anticipated.

The results of this study have prompted the authors to formulate the following conclusions:

1. The ZB2 computer application correctly simulates the process of chemical coagulation of hydrosols.
2. The simulated chemical coagulation proceeds in line with the kinetic equation for a second-order reaction.
3. The simulated sol had the features of a monodispersive sol in the analyzed range of parameters.
4. The variations in the initial velocity of sol particles are induced by the heating or preliminary stirring of sol (eg waste) before coagulation.
5. Excessive heating or stirring of sol (waste) before coagulation is not justified in view of the resulting rate and effectiveness of the coagulation process.
6. The rate of coagulation is insignificantly affected by particle size. The size of sol particles has a greater effect on the coagulation rate than the size of coagulant particles.

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SYMULACJA KOMPUTEROWA PROCESU FLOKULACJI I KOAGULACJI CHEMICZNEJ

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Abstrakt: Opisano wyniki badań przeprowadzonych przy zastosowaniu komputerowego programu „ZB2” symulującego koagulację zawiesiny zawierającej kuliste cząstki zolu i kuliste cząstki koagulantu. Przedstawiono charakterystykę opracowanego programu, a następnie opisano wyniki badań wpływu prędkości początkowej zolu oraz rozmiar cząstki zolu i koagulantu na szybkość procesu koagulacji. Wykazano, iż program „ZB2” pozostaje w zgodności z klasycznymi teoriami ruchu cząstek i destabilizacji układów koloidalnych. Szybkość symulowanego procesu koagulacji, w zakresie opisanym w niniejszej pracy, spełniała równanie kinetyczne II rzędu, a także równanie Smoluchowskiego. Symulowany wzrost prędkości początkowej cząstek zolu zgodnie z oczekiwaniem powodował wzrost szybkości koagulacji. Okazało się także, że większy wpływ na szybkość koagulacji miało zwiększenie średnicy cząstki zolu, aniżeli zwiększenie średnicy cząstki koagulantu.

Słowa kluczowe: koagulacja, flokulacja, symulacja, zol