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EXCESS AND DEFICIENCY OF COAGULANT IN THE COAGULATION PROCESS - COMPUTER SIMULATION

NADMIAR I NIEDOMIAR KOAGULANTU W PROCESIE KOAGULACJI - SYMULACJA KOMPUTEROWA

Abstract: Coagulation is an important process used in water and sewage treatment. Because of its complexity and many factors affecting its speed and efficiency, there is a need for continuous research of a fundamental as well as a utilitarian nature. The kinetics of the coagulation process is still not fully investigated or explained. This is due to the limitations of laboratory experiments, in contrast to computer simulation, which offers practically unlimited experimental possibilities. This paper presents the results of research carried out using a computer program simulating the coagulation of a suspension containing spherical particles of sol and spherical particles of coagulant. The effect of excess and deficiency of coagulant on the formation time of the first flock was identified. The influence of parameters such as the concentration of sol, size of coagulant particles, and the initial velocity of sol and coagulant was analysed. The study revealed that both deficiency and excess of the used coagulant decreased the rate of the coagulation process. It was also found that an increase in the simulated initial velocity of the sol (mixing), as well as the increase in the particle diameter and concentration of the sol increased the speed of sol destabilisation.

Keywords: coagulation, sol, computer simulation

Introduction

Solid pollutants in water and wastewater are usually colloidal and determine turbidity and colour intensity. Coagulation is one of the most effective methods of removing this type of pollution. This process is widely used in the treatment of water and wastewater. However, due to its complexity it continues to be investigated by many scientists [1-4].

Coagulation is a complex physico-chemical process, and its course and efficiency depend on many factors, such as the type and charge of pollutants, pH value, temperature, type and dose of coagulant, reaction time, mixing speed, etc. The range of optimal process conditions is often narrow, *e.g.* with respect to temperature, pH, and coagulant dose, so treatment plants should aim at increasing the range of parameters at which optimal results can be achieved [5]. Computer simulation can help identify correlations between factors affecting coagulation, as it offers practically unlimited experimental possibilities [6-8].

This paper presents the results of research carried out on coagulation and flocculation using a computer program simulating a system containing spherical particles of suspension and spherical particles of coagulant. The effect of excess and deficiency of coagulant on the rate of formation of the first flock was identified. The influence of parameters such as the concentration of the sol, size of coagulant particles, and the initial velocity of coagulant and sol was analysed.

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Materials and methods

The study employed the ZB2 model simulating the process of aggregation, coagulation and sedimentation of spherical sol particles induced by spherical particles of coagulant. The correct operation of this software was proven in previous studies [9, 10]. The ZB2 program is a stochastic-dynamic model. Its operation is based on random variables and the state of the experimental system changes over the simulation time. The core of the program is a module solving the equation of motion for a certain number of points of matter in a closed vessel. The program simulates the process of rapid, perikinetic coagulation wherein each collision of a coagulant particle with a sol particle leads to a stable bond, and particles of the same type do not bind to each other. The coagulation threshold identified as (E) indicates the number of sol particles required to initiate sedimentation; it was determined in such a way that for one particle of the coagulant there is a predefined number of sol particles. The initial values describing the position of particles are generated randomly according to a homogeneous distribution inside the tank. The direction of particle motion and their initial position are selected randomly according to RANDOM instructions. The angle of particle reflection from the wall of the vessel is always equal to the angle of incidence. To simulate the friction between solid particles and liquid, the speed of the flock in the direction of the surface is reduced by 0.1% per shift unit. The sedimentation rate increases with the increase in the number of sol particles in a clump.

In the simulation studies, the following input data were assumed:

N_C - number of coagulant particles; $N_C = 20, 40, 60, 80, 100, 120, 140, 160, 180, 200$
N_S - number of sol particles; in the studies $N_S = 800, 1000$
V_C - initial velocity of coagulant particle; $V_C = 50, 100, 200, 300$
V_S - initial velocity of sol particle; $V_S = 50, 100, 200, 300$
E - coagulation threshold; $E = 10 = \text{const.}$
F - settling coefficient; $F = 0.2 = \text{const.}$
r_C - coagulant radius; $r_C = 1, 2, 5,$
r_S - sol particle radius; $r_S = 1 = \text{const.}$
m_C/m_S - ratio of the coagulant particle mass to the sol particle mass; $m_C/m_S = 1 = \text{const.}$

All measurements of time (t) were taken in seven replicates. Maximum and minimum values were rejected, and the arithmetic mean was calculated for the remaining five values. Values of standard deviation were presented in relevant plots.

Results and discussion

Coagulant dose is an important factor influencing the coagulation process. Excess of coagulant (above a certain optimal dose) is undesirable not only for economic reasons, but it also creates a secondary contamination in the reaction system, which in some cases may pose a greater threat than the substances being removed. For example, aluminium is a typical contaminant used in aluminum-based coagulants, and it remains in the reaction system due to the hydrolysis of the dosed substances. Its content in water during coagulation can significantly exceed acceptable limits.

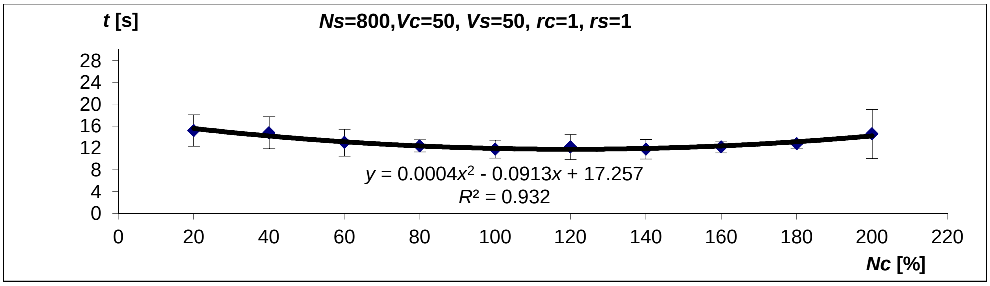

Fig. 1. Effects of deficiency and excess of coagulant on the rate of formation and sedimentation of the first flock

Figure 1 presents the effects of deficiency and excess of coagulant on the time needed for the formation and sedimentation of the first flock, assuming the constant initial velocity of sol and coagulant particles $V_S = V_C = 50 = \text{const}$, and a constant number of sol particles $N_S = 800$. The shortest time for the formation of the first flock was found for the coagulant dose calculated stoichiometrically, *i.e.* at the predefined coagulation threshold ($E = 10$) completely removing particles from the system ($N_C = 100\%$). A significant deficiency of coagulant (20% of the optimal coagulant dose) prolonged the time necessary for the formation of the first flock by 13% compared to the shortest time. As indicated in the figure, both deficiency and excess did not significantly affect the formation of the first flock. It may be expected that a significant excess of coagulant should significantly reduce the time necessary for the formation of the first flock, but the contrary effect was observed, and this time was slightly longer. The excess of coagulant with respect to the assumed coagulation threshold resulted in the dominance of particles with a different charge, and the formation of a new colloidal system under such conditions.

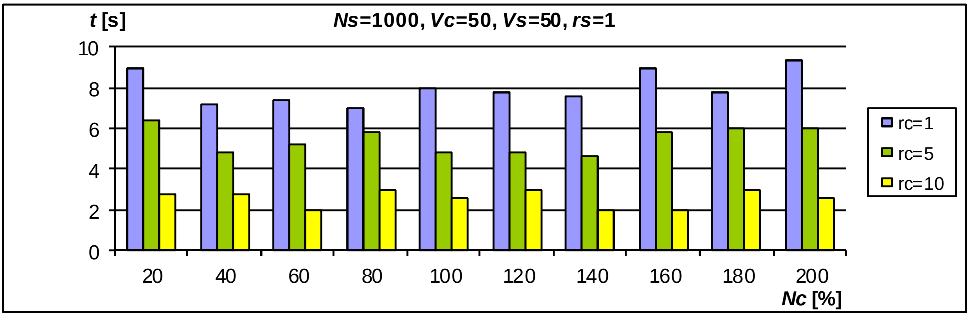

Fig. 2. Effects of deficiency and excess of coagulant of different particle sizes on the rate of formation of the first flock

Another important factor affecting the coagulation process is the type of coagulant. Figure 2 shows the effect of excess and deficiency of coagulant on the time needed for the formation and sedimentation of the first flock at different radii of coagulant particles, *i.e.* 2-, 5- and 10-fold greater than the radius of the sol particle ($r_S = 1$). The increase in the size of coagulant particles significantly reduced the time required to form the first flock.

When coagulant with a radius 10-fold greater than the radius of the sol was used, on average 40% less time was needed to form the first flock compared to the coagulant with a 5-fold smaller diameter. With a 10-fold difference between the radius of the sol particle and coagulant particle, the excess or deficiency of coagulant had no significant effect on the time required for the formation of the first flock. A stronger effect of excess and deficiency of coagulant on the coagulation process was observed for coagulant particles with smaller radii (2- and 5-fold larger than the sol particle radius), and a significant deficiency or excess of coagulant prolonged the time required for the formation and sedimentation of the first flock.

Other important factors influencing coagulation speed are temperature and mixing, which is aimed at the equal distribution of coagulant in the whole volume of water, and ensures the proper course of flocculation.

Figure 3 presents the effect of deficiency and excess of coagulant on the coagulation process. In this case sol particles have a constant initial velocity of V_S = 50, and the initial velocity of coagulant particles is equal to the initial velocity of the sol, or 2-, 4-, or 6-fold higher velocity than the initial velocity of the sol. The presented process simulates preheating or mixing of coagulant before adding it to the sol solution. The figure shows that preheating the coagulant (mixing) has no significant effect on the time required for the formation of the first flock. For the optimal dose of coagulant a 6-fold increase in the initial velocity of coagulant was associated with only a 28% reduction of the time required for the formation of the first flock. The excess of coagulant, regardless of the initial velocity, did not increase the coagulation rate.

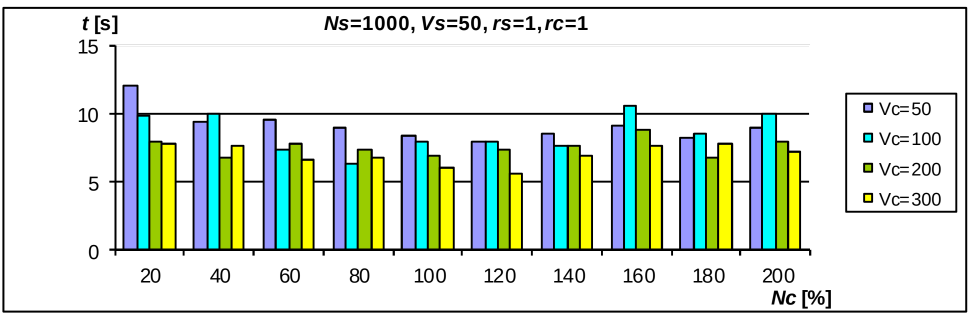

Fig. 3. Effects of deficiency and excess of coagulant of different initial velocity on the rate of formation of the first flock

Figure 4 shows the effects of excess and deficiency of coagulant under simulated conditions where the sol solution was preheated (mixed) before adding coagulant; sol particles had an initial velocity 2-, 4-, or 6-fold greater than the initial velocity of coagulant, *i.e.* V_C = 50 = const. Figure 5 presents the effects of deficiency and excess of coagulant on the simulated coagulation where coagulant and sol particles had the same initial velocity. Figures indicate that the coagulant dose can be significantly reduced by increasing the initial velocity of sol to achieve the desired coagulation rate. The coagulation rate increased with the increase of the initial velocity of either sol particles alone (Fig. 4) or sol and coagulant particles (Fig. 5). For the optimal dose of coagulant a 6-fold increase in the initial velocity of sol and coagulant reduced the time required for the formation of the first flock by 64%. At 4- and 6-fold increases of initial velocity the deficiency or excess of coagulant had no significant effect on the formation time of the first flock.

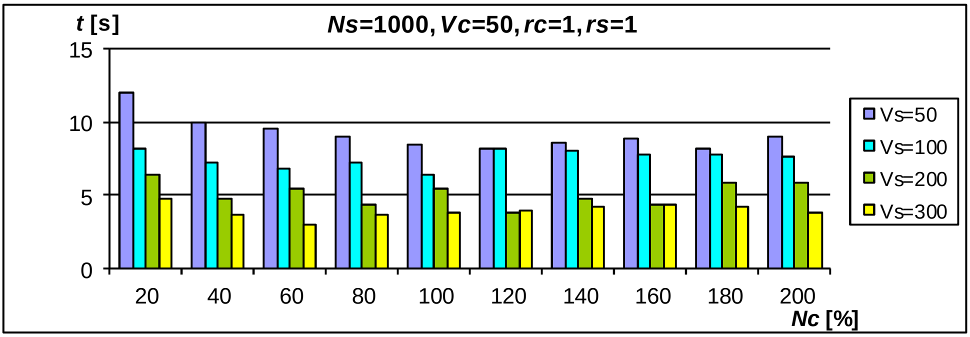

Fig. 4. Effects of deficiency and excess of coagulant with the constant initial velocity of coagulant particles and increasing initial velocity of sol on the formation time of the first flock

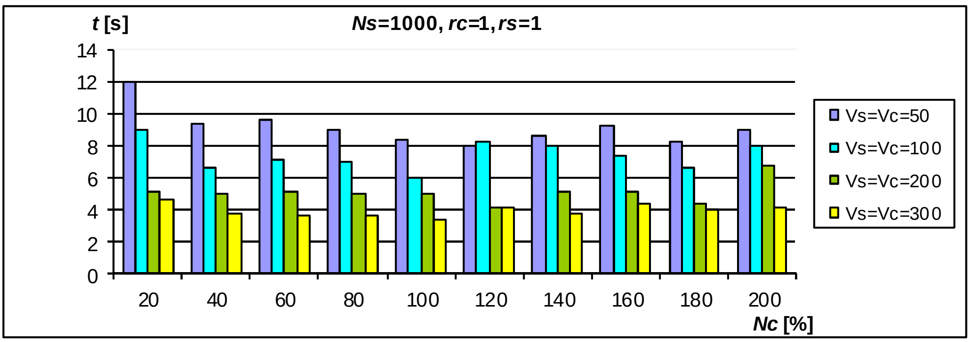

Fig. 5. Effects of deficiency and excess of coagulant with the increasing initial velocity of coagulant and sol particles on the formation time of the first flock

Summary and conclusions

Coagulant dose is an important factor affecting coagulation, and both its deficiency and excess may have a negative impact on coagulation. In the presented simulation model coagulation was achieved through the interaction of two colloidal systems, sol and coagulant. Both deficiency and excess of coagulant reduced the coagulation rate. Equal or close to equal absolute values of two opposite charges of both sols are necessary for coagulation. If one of the sols is present in excess or is deficient, then coagulation may be partial or fail completely. Colloids with opposite charges adsorb each other, and the charge that has not been neutralised remains on a newly formed particle. If coagulation occurs in two interacting colloidal systems, then the excess of coagulant above the predefined coagulation threshold causes the dominance of particles with the opposite charge and a new colloidal system is formed.

The type of coagulant in the simulated system and increase in the size of coagulant particles increased the coagulation rate. The effect of excess and deficiency of coagulant on the coagulation process was much weaker for coagulant particles with a longer radius (10-fold greater than the sol particle radius) than for coagulants with shorter radii (2- and 5-fold greater than the sol radius), where a significant deficiency or excess of coagulant prolonged the time required for the formation of the first flock.

Coagulation conditions, preheating or mixing of the coagulant before adding it to the sol solution had no significant impact on the coagulation rate. However, preheating and mixing of the sol before adding coagulant had a significant impact on the formation of the first flock and coagulation rate. For sol particles with a higher initial velocity the deficiency or excess of coagulant has no significant effect on coagulation rate. A coagulant dose can be considerably reduced by increasing the initial velocity of sol, and the desired coagulation rate is still achieved.

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NADMIAR I NIEDOMIAR KOAGULANTU W PROCESIE KOAGULACJI - SYMULACJA KOMPUTEROWA

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Abstrakt: Koagulacja jest istotnym procesem stosowanym w oczyszczaniu wody i ścieków. Jest to proces złożony, wiele czynników wpływa na jego szybkość i efektywność. Stąd wynika potrzeba ciągłych badań natury zarówno fundamentalnej, jak i utylitarnej. Kinetyka procesu koagulacji ciągle pozostaje nie do końca zbadana i wyjaśniona. Wynika to z ograniczeń w obszarze laboratoryjnego eksperymentowania, w przeciwieństwie do symulacji komputerowej, która praktycznie stwarza nieograniczone możliwości eksperymentalne. W pracy przedstawiono wyniki badań przeprowadzonych przy zastosowaniu programu komputerowego symulującego koagulację zawiesiny zawierającej kuliste cząstki zolu i kuliste cząstki koagulantu. Określono wpływ nadmiaru i niedomiaru koagulantu na szybkość tworzenia pierwszego kłaczka. Badano wpływ takich parametrów, jak stężenie zolu, rozmiar koagulantu, prędkość początkowa koagulantu i zolu. Stwierdzono, że zarówno niedomiar, jak i nadmiar stosowanego koagulantu powodował obniżenie szybkości procesu koagulacji. Stwierdzono także, że wzrost symulowanej prędkości początkowej zolu (mieszanie), wzrost średnicy i stężenia zolu powodował wzrost prędkości destabilizacji zolu.

Słowa kluczowe: koagulacja, zol, symulacja komputerowa