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Modeling of the Distribution of Electric Discharge Between Metal Balls in the Aqueous Solution

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In this work it is planned to apply the MPC approach for the optimization of energy consumption of electroerosion process for water purification. For this purpose is necessary to develop a mathematical model of the water purification process. Distribution of electrical discharges between the metal balls in contaminated water is one of the stages of electroerosion process for water purification. In this paper a mathematical model of the distribution of electrical discharges between the metal balls in the aqueous solution is presented. Method of probabilistic cellular automata was used to develop a mathematical model, since the distribution of electrical discharges is a stochastic character. The modeling results were compared with experimental data.

1. Introduction

Nowadays, the tasks of creation and upgrading of technologies and methods for the purification of air and water from pollution are of scientifically interest. CO_2 emissions in the atmosphere are increasing due to the large use of natural gas and coal for the production of electric energy. Reducing CO_2 content in the atmosphere is an actual problem. Azmi et al. (2016) proposed a combined process of adsorption and gas hydrate formation as an alternative approach for the separation of carbon dioxide (CO_2) content from gas stream. The objective of this research was to study adsorption isotherms of the CO_2 onto the synthesized calcium oxide (CaO) via a static volumetric method at 2 °C and at different amount of water ratio. Zarogiannis et al. (2016) studied a systematic approach for the preliminary screening of binary amine mixtures as CO_2 capture candidates considering several important properties as selection criteria. A study of the population of any country with quality classification of drinking water and the treatments used for industrial wastewater is also an urgent task. Today a large number of water purification methods are used: reverse osmosis, reagent coagulation, aeration, sedimentation, distillation, etc. Each of the foregoing methods have different advantages and disadvantages. Lutchmiah et al. (2014) reviewed problems and prospects the use of reverse osmosis membranes for wastewater treatment. The main disadvantages dealing with these methods are: a large consumption of reagents, the need for periodic replacement of membranes, high costs of reagents and membranes, large areas needed for equipment installation and the ineffectiveness to clean water sources by toxic substances, like arsenic, and dissolved salts. In the scientific literature, several articles studied different optimization approaches and the development of automatic control systems. In the study of Manenti et al. (2015) an optimization work on the reverse osmosis module with recycle is developed using MPC approach. However, the proposed control and optimization system cannot eliminate the disadvantages inherent to these methods. Therefore, it is necessary to develop a new energy-saving and resource-efficient methods for water purification.
One of these methods, based on the use of electric energy, is the water purification by electroerosion process (EDM process) of metal balls. The electroerosion process of metal workpieces has been known for more than 70 years, but the use this method for water purification is a novelty. This new process of electroerosion for water purification has several advantages: it is based on cheap raw materials (metal balls) and characterized by low energy consumption. Since this is a new and poorly known method, it is necessary the study of a suitable

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mathematical model for the optimization and the development of a control system. The MPC approach for development of control systems was applied.
The mathematical model of the process is necessary for modeling, optimization and development of control systems based on the predictive model. There are papers devoted to the modeling electrical discharge machining (EDM) of metal products by using machines, as well as papers devoted to the modeling individual stages of the electric erosion process. Wuyi Ming et al. (2014) proposed, for electrical discharge machining process, a hybrid intelligent process model, based on finite-element method and Gaussian process regression. In order to predict material removal rate and surface roughness a model of single-spark EDM process has been done based on finite-element method, considering: the latent heat, the variable heat distribution coefficient of cathode and the plasma flushing efficiency. However, these models are not suitable for the simulation of electroerosion process for water purification, because there is a difference in the distribution of the discharge energy, and consequently in the products erosion formation. The aim of this paper is to develop a mathematical model of distribution of electrical discharges between the metal balls in the aqueous solution.

2. Process description

The electroerosion process for water purification is only one stage of technological process of water purification from contaminants. The main destination of this method is that convert soluble salts into insoluble precipitate that can be easily removed from water. The scheme of water purification is shown in Figure 1.

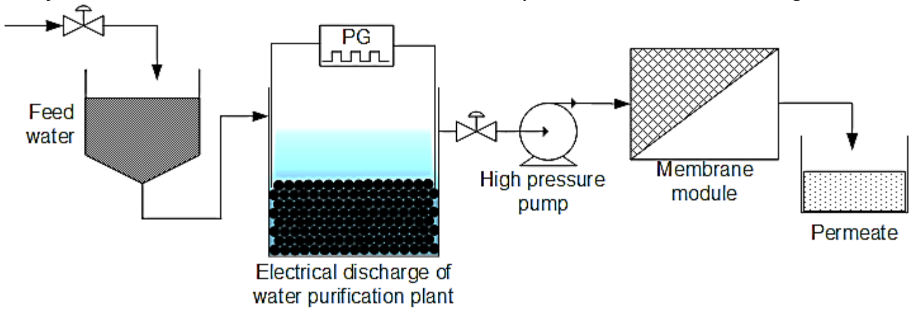


Figure 1: Possible technological scheme of the water purification plant

Technological scheme (see Figure 1) includes a tank with feed water, electrical discharge (electro erosion) of water purification plant, high pressure pump, membrane module for filtration of erosion products from water. The membrane module may be replaced by a settler tank in which the electroerosion products can be deposited. It will allow reduce the cost of water purification, but will worsen the degree of water purification.
In this paper was discussed processes in the electrical discharge in water purification plant. The electrical discharge equipment of water purification plant consists of electrical pulse generator (PG) and the tank-reactor Two electrodes are located in the reactor-tank and connected to the PG. The interelectrode gap, in the tank-reactor, is filled with metal balls and purified water. Then, electrical impulses of short duration passed through the layer of metal balls. Electrical discharges arise between the balls when the electrical impulses pass. These discharges are characterized by high energy. As a result, electrical erosion process occurs on the surface of metal balls. The separated erosion products are highly dispersed particles of metal. The size of the dispersed particles is about 1 - 100 nm. Nadezhdin et al. (2016) presented the mathematical model and the mechanism of formation of electroerosion holes and electroerosion products.
The erosion products were oxidized by water. As a result, metal hydroxides and oxides were formed and were active coagulants. The formed metal hydroxides and oxides efficiently adsorbe impurities contained in water and form insoluble salts that can precipitated. Nadezhdin et al. (2016) presented the chemical reactions that describe chemical processes occurring in the tank-reactor and a mathematical model able to describe chemical reactions kinetic of electroerosion process for water purification.
The optimum power of electrical pulses can be determined. The maximum amount of erosion products is formed as result of these impulses. This will optimize the energy consumption of electroerosion process for water purification. The task of increasing the electrical discharges between balls ("tracks" discharges) as result of one electrical impulse arises. The mathematical model of the distribution process of electrical discharges between the metal balls into aqueous solution is planned to be applied to optimize.

3. Mathematical modeling of the distribution of "tracks" discharges

3.1 Application of probabilistic cellular automata for modeling of "tracks" discharges

Place initiation and trajectory of the distribution of electrical discharges between the metal balls in the interelectrode gap of the electrical discharge have a stochastic character. Method of probabilistic cellular automata was used to develop a mathematical model of distribution of electrical discharges between the metal balls ("tracks" discharges). The metal balls are located in layer a certain height in the plant, depending by the backfilling mass. As can see in Figure 2, one ball is adjacent to 6 balls from its layer and to 3 from above and below layer. Thus, one ball in the plant may have up to 12 of adjacent balls.

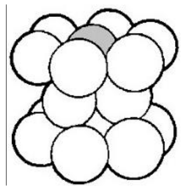
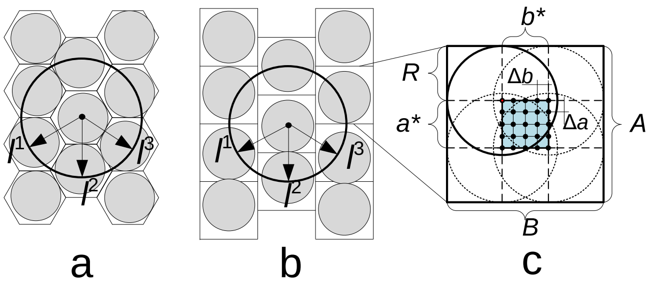


Figure 2: Location of metal balls in tank of the electrical discharge of water purification plant

Considering each layer, the balls separately it can be seen that the distribution of balls satisfies of the hexagonal lattice cellular automata, which shown in Figure 3a. The metal ball is located in each cell of the hexagonal lattice (see Figure 3a). The hexagonal lattice is undergoing certain transformations for computer implementation (see Figure 3b). The cells of lattice can take on two values during modelling. The first value indicates that the discharge has passed through the cell (the ball), the second value indicates that the cell (the ball) was not exposed to electric discharge.



a) the initial hexagonal lattice; b) lattice, which being implemented in a computer; c) scheme for determining the position of the ball in the cell

Figure 3: Location of metal balls in the layer of the backfilling

The interelectrode gap is represented as a series-parallel circuit of the resistors. The metal balls and aqueous solution filling the space between the electrodes are represented as a circuit of resistors. Between the balls there is a thin film of water, regardless of as tightly they are adjacent to each other (about 1 µm). Distribution of electrical discharges between the metal balls depends by the thickness of the water film between balls. The thinner the film of water, the smaller the resistance. The electrical discharge is distributed along the path with the least resistance. The thickness of the water film between the balls depends on the location of the balls in the plant. The balls are arranged in an arbitrary way in the apparatus. Some balls are more firmly pressed to each other. Accordingly, between them is smallest thickness of the water film. The balls are misaligned in the some direction while located in cells of the hexagonal lattice. In addition, the presence of "tracks" discharges between the potential electrode and the balls is a random process. This process is dependent on the location of the balls in the plant. Initially defined by a limiting distance between potential electrode and balls in the near to it row ($l_{\text{el-ball}}$). If the distance between electrode and balls is less than the specified ($l_{\text{el-ball}}$), then there is the breakdown. Thus, emerging as much of "tracks" discharges, as much as balls located at a distance of less $l_{\text{el-ball}}$ from the electrode. Balls location in the plant has a stochastic character. It is assumed that the center of each ball can be in some permissible region $a^* \times b^*$ (see Figure 3c). The dimensions of this region are defined by using the following expressions:

$$a^* = A - d_{ball},\ A = d_{ball} + l_{film} \ \ and \ \ b^* = B - d_{ball},\ B = d_{ball} + l_{film} \tag{1}$$

where A, B is parameters dependent on the thickness of the water film between the balls (mm); l_{film} is the thickness of the water film between the balls (mm), about 10^{-3} mm. Further, given by the number of possible positions of the center ball in this region, Δ_a and Δ_b are calculated by using the following Eq(2)

$$\Delta a = a^* / n_a^{\max} \quad and \quad \Delta b = b^* / n_b^{\max} \tag{2}$$

where $n_a^{\max}$ and $n_b^{\max}$ are the maximum number of possible positions of the center ball in the allowable region $a^* \times b^*$. Placing of the center ball in the one of the possible positions is performed using a function that returns two random integers from 0 to $n_a^{\max}$ and $n_b^{\max}$, which specify the coordinates of the center ball in region $a^* \times b^*$.

3.2 The mathematical model of the distribution of "tracks" discharges

The number of balls in one layer of backfilling and height of the entire layer of backfilling in the plant are necessary to understand how to determine the trajectory and the number of "tracks" discharges. Height of the entire layer of backfilling in the plant is calculated with the Eq(3)

$$h_{\text{layer}} = N_{ball} / N_{ball}^1 \tag{3}$$

where N_{ball} is the number of balls in the backfilling (pcs); N_{ball}^1 is the number of balls in one layer of the backfilling (pcs). The number of balls in one layer of the backfilling can be found by using the Eq (4):

$$N_{ball}^1 = l_{pl} \cdot w_{pl} / d_{ball}^2 \tag{4}$$

where d_{ball} is diameter of the balls in backfilling (mm); l_{pl} is length of the plant (mm); w_{pl} is width of the plant (mm). The number of balls in backfilling is determined using the Eq(5)

$$N_{ball} = m_{fill} / m_{ball} \tag{5}$$

where m_{fill} is mass of backfilling (kg); m_{ball} is mass of one ball (kg). The mass of one ball can be determined using Eq(6)

$$m_{ball} = V_{ball} \cdot \rho_{ball} = \frac{4}{3} \cdot \pi \cdot R_{ball}^3 \cdot \rho_{ball} \tag{6}$$

where V_{ball} is volume of ball (m^3); ρ_{ball} is density of ball (kg/m^3); R_{ball} is radius of ball (m).
As said earlier, the number of arising "tracks" discharges, depends on the number balls located at a distance of less $l_{el\text{-}ball}$ from the electrode. Electric current flow through the least resistance path. One of the parameters of each cell is the conductivity of the film water. The conductivity of the film of water determines the current flowing between the two balls of backfilling, and it is defined by the formula Eq(7), which follows from Ohm's law:

$$I = U \cdot S \cdot \gamma / l_{ball-ball} \tag{7}$$

where I is current of conduction (A); U is voltage of pulse (V); S is sectional area of channel (m^2); γ is electrical conductivity of the aqueous solution ($\Omega^{-1} \cdot cm^{-1}$); $l_{\text{ball-ball}}$ is distance between the balls.
The balls have a probabilistic character of the distribution in the plant, so the distance between ($l_{\text{ball-ball}}$) the balls is arbitrary values, thereby changing the resistance of part an electrical circuit (of water film). Since the distribution of discharges is due to potential electrode and ground electrode, then discharge has three potential areas for further spread in balls layer (see Figure 3a,b). The following conditions are checked to find the minimum distance between adjacent balls:

$$\begin{cases} l_{ball-ball}^1 < l_{ball-ball}^2 \ \& \ l_{ball-ball}^1 < l_{ball-ball}^3 \\ l_{ball-ball}^2 < l_{ball-ball}^1 \ \& \ l_{ball-ball}^2 < l_{ball-ball}^3 \\ l_{ball-ball}^3 < l_{ball-ball}^1 \ \& \ l_{ball-ball}^3 < l_{ball-ball}^2 \end{cases} \tag{8}$$

finding the minimum distance ($l_{ball-ball}^i = l_{ball-ball}^{\min}$) appropriate cell changes its state and process is repeated until the ground electrode is not reached. The length of "tracks" discharge depends by electric field intensity (E) in the interelectrode gap. The electric field intensity decreases by the exponential law. The electric field intensity takes a value less than value of the critical intensity (E_{crit}) at a certain distance from the potential electrode. When $E<E_{crit}$ breakdown of the water film between the metal balls did't happen and part of the backfilling takes the role of the ground electrode. The length of the "track" discharges in interelectrode gap is calculated Eq(9)

$$l_{"track"\ disch} = {-a \cdot l_{\text{interel.}}^{b}} \Big/ {\ln\left(1-\frac{E_{crit}}{E_0}\right)} \tag{9}$$

where a = 31.93 and b = 0.0204 are empirical coefficients; $l_{interel.}$ is length of the interelectrode gap (mm); $E_0 = U/l_{el-ball}$ is the electric field intensity near the surface of potential electrode (V/mm); $l_{el\text{-}ball}$ is the distance between the electrode and the nearest hall, about 0.001 mm. Equation (9) was obtained by the analysis of experimental data. The critical electric field intensity is calculated by using of the empirical formula Martin Eq(10):

$$E_{crit} = A \Big/ \left(t_{on}^{1/3} \cdot S_{el.}^{1/10}\right) \tag{10}$$

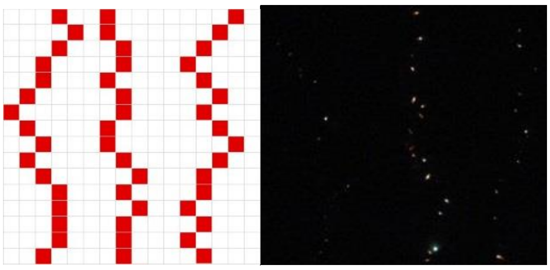
In Eq.(10), A is an empirical constant (for water is 0.6 MV/cm in case of breakdown with cathode or 0.3 MV/cm in case of breakdown with anodo); t_{on} is the electric pulses duration (µs); $S_{эл}$ is area of the electrodes (cm^2). The developed model allows the calculation of the number and the length of the "tracks" discharges, occurring as a result of the electrical pulses. Changing of the mass of metal balls have been loaded in the water purification plant is determined according Eq (11)

$$\frac{dm_{fill}}{dt} = m_{fill} - m_{Fe}^{ЭЭО} \tag{11}$$

where m_{Fe}^{EDM} is the formed electroerosion products mass (kg). A mathematical model for the calculation of the formed electroerosion products mass gas presented by Nadezhdin et al. (2016).

4. Results and discussions

The mathematical model developed was implemented in the form of program code. Modeling and experimental research were carried out with the following parameters: d_{ball} = 6 mm, w_{pl} = 100 mm, $l_{pl1} = l_{interel1}$ = 180 mm, $l_{pl2} = l_{interel2}$ = 100 mm, $n_a^{\max} = 8$ and $n_b^{\max} = 8$, weight backfilling is: m_{fill1} = 0.430 kg, m_{fill2} = 0.230 kg. Metal balls were distributed in the tank in one layer at a given amount of backfilling. Electric pulses of duration t_{on} ≈ 25 µs and amplitude U = 500 V were passed through a layer of balls. The obtained results are shown in Figure 4.



The distance between the electrodes is 100 mm

the distance between the electrodes is 180 mm

Figure 4: The modelling results and photos of the interelectrode space

As seen from the images (see Figure 4), modeling was performed for the electrode gap of different lengths. Electrical discharges did't reach the ground electrode when distance between the electrodes is increased, since the electric field intensity was insufficient. During the research, 30 experiments were performed for each interelectrode gap. The number of "tracks" discharge was different each time. The obtained results are presented in Table 1.

Table 1: The data of experiments and modeling

The number of "tracks" discharge	The length of the distance between electrodes, mm			
	100		180	
	The probability of occurrence, %		The probability of occurrence, %	
	Model	Experiment	Model	Experiment
2	10.0	10.0	73.3	66.6
3	70.0	73.3	20.0	26.7
4	13.3	16.7	6.7	6.7
5	6.7	3.3	0	0

Experimental results shows that a number of "tracks" discharge equal to three is characteristic for an interelectrode distance of 100 mm while increasing the interelectrode distance at 180 mm the number depresse at two (see Table 1). Discrepancy between the experimental and computational data for the 100 mm of interelectrode gap is equal 3.4 % and for the 180 mm of interelectrode gap is equal 5.2 %.
As can be seen from the obtained data (see Figure 4 and Table 1) not all the balls are processed case of insufficient power electric pulses. Accordingly, the number and length of the "tracks" discharge is decreases. Surplus energy is spent on heating the water in the plant when the power of electric pulses have too large values. Therefore, the determination of the electrical pulses optimal power is also an important task. For solve this task, planned to use mathematical model developed in this research.

5. Conclusions

In this paper was presented a mathematical model of the distribution of electrical discharges between the metal balls in the aqueous solution. During the research was proposed a new approach to the modeling of the distribution of electrical discharges between the metal balls in the interelectrode gap in the water purification process. The proposed approach was based on the use of probabilistic cellular automata. Therefore, in the paper was reported an empirical relationship length of "tracks" discharge on the electric field intensity in the interelectrode gap. The modeling results were compared with experimental data. The discrepancy between the data was about 5 %. Obtained data confirm the adequacy of the developed model and allow to use it in the further work.

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