Representation of the galvanic coagulation process using a mathematical model

A S Kozodaev¹,², A D Shulzenko¹,* and Y V Korpusova¹

¹ Department of ecology and industrial safety, Bauman Moscow State Technical University, 5/1, 2ya Baumanskaya st., Moscow, 105005, Russia
² Department of environmental engineering and labor protection, Moscow Power Engineering Institute, 14 Krasnokazarmennaya str., Moscow, 111250, Russia

*annadmitrevnash@mail.ru

Abstract. This work is devoted to the study of the process of water purification by galvanic coagulation. It is known that this method is promising for the extraction of toxic contaminants such as heavy metals from wastewater. However, there are no techniques or mathematical dependencies to simulate the treatment process. The paper investigated the chemical side of galvanic coagulation, and also proposed a mathematical model based on a two-stage chemical reaction model and a metal electrochemical corrosion model.

Anthropogenic impact on the environment as a result of irresponsible human activity has reached a critical value. The danger of global environmental problems is that their aggravation poses a threat to human health, life [1].

The protection of water resources from depletion and pollution and their rational use for the needs of the national economy is one of the most important problems requiring urgent solutions[2].

Due to the huge number of various industries, discharged waters are often polluted with a large variety of pollutants including organic pollutants, petroleum products, heavy metals, and others [3-6]. For example, wastewater from electroplating plants is one of the main anthropogenic sources of heavy metal ions into natural water bodies [7].

Up to 52 cubic kilometers per year of wastewater are discharged into water bodies of the Russian Federation, of which 19.2 cubic kilometers are subject to treatment.

Together with wastewater, about 11 million tons of pollutants enter the surface water bodies of the Russian Federation annually [8].

In this regard, wastewater treatment is an important practical task.

Today, there is various equipment aimed at preventing the release of these components into the environment. Among a wide range of physicochemical methods of wastewater treatment, the method of galvanic coagulation is of wide interest. It belongs to electrochemical processes, which are distinguished by their instrumental simplicity and high purification efficiency.

The method of galvanic coagulation is considered economical since it does not require expensive reagents and is characterized by low power consumption [9]. In contrast to electrochemical methods, it is easy to maintain, highly reliable, and can be used as reagents from residues from other industries.

In the galvanic coagulation method of water purification, when heterogeneous particles come into contact, a short-circuited galvanic cell is formed, where a more electronegative metal dissolves.
Accordingly, a colloidal hydroxide is formed, which has good adsorption capacity and is the main water treatment agent.

The interaction of the metal and the resulting colloidal hydroxide can be described by a number of reactions using aluminum as an example:

1) Dissolution of the anode followed by the formation of hydrate ions $\text{Al}^{3+}$;
2) Oxidation of water molecules

$$2\text{H}_2\text{O} \rightarrow \text{O}_2 + 4\text{H}^+ + 4\text{e}$$ (1)

3) Dissolution of the protective film of aluminum oxide

$$\text{Al}_2\text{O}_3 + 6\text{H}^+ \rightarrow 2\text{Al}^{3+} + 3\text{H}_2\text{O}$$ (2)

4) Chemical relationship of aluminum with water

$$2\text{Al} + 6\text{H}_2\text{O} \rightarrow 3\text{H}_2 + 2\text{Al(OH)}_3$$ (3)

The resulting hydroxide, by coagulation, forms insoluble compounds with heavy metals, which precipitate faster and are easily dehydrated [10].

Previous experimental studies [11] confirm the rationality of research and further use of the method of galvanic coagulation treatment. However, for the effective application of this method in practice, the problem of its modeling is urgent.

Within the framework of this work, the process of water purification is considered as the two-stage process of an ideal mixing reactor, shown in Figure 1.

![Figure 1. Model of a chemical reaction.](image)

Stage A – implies a state when pollution is bound in the formed hydroxides. It is characterized by the concentration of pollutants in the CA water.

Stage B is considered a state in which contaminants are adsorbed by a freshly formed coagulant. It is characterized by the concentration of the extracted contaminants CB.

The wastewater treatment process in a galvanic coagulator is considered as a dynamic model of an isothermal ideal mixing reactor of continuous operation. Accordingly, the mathematical model of an ideal mixing reactor will have the following form (2.83 p. 65 [12]):

$$\frac{dC_A}{dt} = -kC_A, \quad \frac{dC_B}{dt} = kC_A$$

The constants $k_1$ and $k_2$ determine the intensity of the transition between the states – the rates of the forward and reverse reactions. The process of decomposition of the formed aggregates based on insoluble hydroxides is unlikely; therefore, the reverse reaction is not considered.

Further, the parameters most strongly influencing the reaction rate were identified. Therefore, the constant k is the following relationship:
where \( v_{Al(OH)_3} \) – is the rate of hydroxide formation; \( m_{H_2O} \) – is the mass of water involved in the treatment.

The mass of purified water is considered through the flow passing through the galvanic coagulator:

\[
m_{H_2O} = Q t \rho,
\]

The rate of formation of hydroxide directly depends on the rate of oxidation of aluminum in water – that is, on the rate of electrochemical corrosion of the metal of the galvanic couple. Accordingly, we accept the simplification that the rate of formation of hydroxide is equal to the rate of corrosion of aluminum. Therefore, this parameter of the constant is revealed through the indicators of corrosion: weight and current \([13, 23]\). Using the formulas of these parameters, we get an expression describing the mass of the oxidized metal in time \([13-24]\).

\[
v_{Al(OH)_3} = \frac{\Delta m}{t} = \frac{i M S}{n F},
\]

where \( i \) – is the current indicator of corrosion; \( M \) – is the molar mass of the metal; \( S \) – is the area of the contacting surface; \( F \) – is the Faraday number; \( n \) – is the number of moles of electrons.

The current index is considered as the density of the corrosive current \([13, 14, 16-19]\):

\[
i = \frac{\Delta \varphi}{S(R+R_K+R_A)},
\]

where \( \Delta \varphi \) – is the potential difference between the cathode and the anode; \( R \) – is the resistance of the electrolyte between the elements of the galvanic couple; \( R_K \) – is the resistance arising due to the polarization of the cathode; \( R_A \) – is the resistance arising due to the polarization of the anode.

The resulting constant takes the following form:

\[
k = \frac{\Delta \varphi M S}{(R+R_K+R_A)n F Q t \rho} = \frac{\Delta \varphi M}{(R+R_K+R_A)n F Q t \rho}
\]

In this case the system (1) becomes the following form:

\[
\begin{align*}
\frac{dC_A}{dt} &= -\frac{\Delta \varphi M}{Q t (R+R_K+R_A)n F} C_A, \\
\frac{dC_B}{dt} &= -\frac{\Delta \varphi M}{Q t (R+R_K+R_A)n F} C_A \\
\end{align*}
\]

The initial conditions are imposed on this mathematical model: \( t = 0, C_A = C_{A0}, C_B = 0 \).

Conclusion

- In this paper, we proposed a mathematical model that solves the problem of determining the required treatment time to achieve a sufficient level of extraction of heavy metals from the wastewater.
- The main parameters affecting the process rate were identified and substantiated.
- A numerical analysis is planned for the model in the future.

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