Numerical simulation of the preparation of a compounded oil pitch with reduced carcinogenic activity

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Abstract. The paper presents a numerical simulation of the preparation of a compounded oil pitch, which, in addition to high technological parameters, has high environmental indicators. Environmental friendliness is ensured by the low content of harmful impurities, including carcinogenic benzo (a) pyrene.

1. Introduction

Along with increasing the efficiency of energy-intensive metallurgical industries, the trend in the development of world industry is to improve the environmental performance of these enterprises. Primary aluminum production volumes are growing from year to year, despite the controversial situation in the global economy. Aluminum is the basis of most of the most popular alloys and composite materials, the need for which is increasing every year. Modern Russian science is making great strides in the study of alloys and composite materials [1-6].

In addition to the main products of metallurgical production, a promising area of research is the isolation and use of materials released along the way with the high-energy metallurgical process [7,8]. Such materials are various nanostructures and nanomaterials formed in the form of nanosized particles discharged to the gas treatment system of a metallurgical enterprise [9]. Materials obtained from these nanostructures are used in concrete, rubber products, alloys, etc. [10].

Russia is one of the leaders in primary aluminum production. This position in the world market obliges to comply with international environmental standards. Despite the development of electrolysis technology using calcined anodes [11–13], primary aluminum obtained by the Söderberg technology has the lowest cost. To date, this technology is used in large Russian factories and reducing environmental impact is an urgent task.

In the process of aluminum electrolysis, there are a number of technological processes during which the largest amount of harmful substances is released into the environment. These processes include the following:

- stationary (interoperational) mode. Despite the fact that this mode is environmentally optimal (regular operation of the suction system, closed shelters, etc.), the stationary mode is the main time for aluminum electrolysis and it is in this mode that there is great potential for improving environmental performance [14-16].
- pouring;
- change of anode pins;
- as well as other operations related to routine maintenance.
The basis for the production of primary aluminum using Söderberg technology is the use of self-baking anodes, the most active and unsafe component of which is the binder. The environmental properties of the binder have a great impact on the overall ecology of aluminum production.

2. Materials and research methods

Modeling the process of compounding an oil binder with carbon nanostructures is necessary to assess the design of the reactor, high-speed mixing modes, as well as temperature and other technological parameters. Modeling was carried out on the material and technical base of the Federal State Budget Educational Establishment of Higher Education "Irkutsk National Research Technical University".

Fluid circulation and tracking the trajectories of particles entering the mixed fluid were estimated by means of numerical simulation in Ansys software based on the finite volume method.

General characteristics of the model:
- 251 thousand settlement nodes;
- turbulence model - k-omega SAS;
- the geometry of the computational domain is shown in Figure 1;
- the blades of the mixing device in the form of an inverted trapezoid.

Mixing medium parameters:
- density 1000 kg / m³;
- dynamic viscosity 1.75 P (Poise, 175 centipoise);
- temperature 150 °C (the method of temperature selection is given below);

the ratio of the binder to carbon nanomodifier was selected during the search experiments and amounts to 10 parts of the binder to 2 parts of the modifier, which is the maximum estimated amount of additive.

3. Results and Discussion.

The temperature of the mixing medium was determined empirically, in order to save time on numerical simulation, based on the current parameters of the laboratory mixing device - at a temperature of 150 °C the ratio of revolutions and current of the mixer comes to the nominal, this means that further heating does not make sense, and this temperature is minimum sufficient.

![Figure 1. The geometric shape of the computational domain of numerical simulation.](image)

The shape of the container is selected in the form of a smooth cylinder with a height of about two diameters. The mixing device is selected with the aim of organizing a downward funnel-like flow, which allows the upper layers of the mixed medium to be pulled down.
At the set temperature and concentration of solid particles, the most important parameter is the speed of rotation of the mixing device. In order to optimize this mixing parameter, modeling was carried out in three different speed modes:

- 200 rpm;
- 400 rpm;
- 600 rpm;

At all these speeds, the particles of the modifying additive were fed onto the surface of a binder heated to a temperature of 150 °C. Figures 2 – 4 show the results of modeling the mixing process for speeds of 200 rpm, 400 rpm, 600 rpm, respectively.

**Figure 2.** Simulation results at a stirrer speed of 200 rpm.

**Figure 3.** Simulation results at a stirrer speed of 400 rpm.
Figure 4. Simulation results at a stirrer speed of 600 rpm.

From the above simulation results, we can draw the following conclusions:

- at a rotation speed of the mixing device of 200 rpm (obviously at a lower speed), the particles, and therefore the mixing medium, do not develop the speed necessary for uniform distribution of particles in the reactor volume;
- at a rotation speed of the mixing device of 400 rpm, a fairly uniform distribution of particles in the medium is observed, no negative effects are observed;
- at a rotation speed of the mixing device of 600 rpm (obviously at a higher speed), the particles of the modifier are separated by hydraulic fineness, which leads to the separation of particles in the reactor chamber. In addition, a high rotational speed can in practice lead to foaming or spraying of a substance.

The mixing speed was adopted 400 rpm as the most optimal according to the simulation results.

Figure 5 shows the simulated motion paths of individual particles of solid material at a stirring speed of 400 rpm, with a stirring time three times longer than in the simulation version shown in Figure 5.2. As can be seen from Figure 6, a high degree of uniformity of mixing was achieved.

Figure 6 shows the trajectories of particles falling onto the surface of the liquid by top loading into the reactor. The starting point is at the top, from where they go down along the wall and to the center, then again down along the walls. From this model, we can conclude that the top load will achieve high-quality mixing.

From Figure 6 it can be seen that the introduced material is drawn into the mixing zone together with the fluid flow. Thus, to ensure mixing of a sufficient degree of uniformity, it is necessary to choose the mixing time. No special requirements for the shape of the blades of the mixing device have been identified, the presence of inclined surfaces for the formation of vertical circulation is sufficient.
Figure 5. Trajectories of solid particles in a mixing reactor according to the results of numerical simulation.

Figure 6. Trajectories of solid particles in a mixing reactor according to the results of numerical simulation.

4. Conclusion
The optimal mixing parameters according to the results of numerical modeling: temperature 150 °C, rotation speed of the mixing device 400 rpm, top loading of the material. With these parameters, the most optimal mode of obtaining a compounded oil pitch with high environmental performance is expected. This material will be of high importance for the environmental component of primary aluminum production in Russia.
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