Modeling of the Ions Streams by the Method of Particles

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Abstract. The work is devoted to modeling of flows of the charged particles in an electrostatic field arising in the course of electrolysis between a surface of the cathode and the anode. The mixed method of particles adapted for modeling of the migratory diffusion of a stream of ions in the course of electrolytic refinement is given in the article. At the Eulerian stage potentials of an electrostatic field are modelled by means of Maxwell's equations. At the Lagrangian stage the motion laws and trajectories of ions are developed in the form of the square-law splines . The results of computer modeling for the electrolytic refinement of copper are given.

Keywords: method of particles, Maxwell's equations, electrolytic refinement, square-law spline, mathematical model, migratory diffusion

1 Introduction

The investigation of ions streams in the electrostatic fields is rather actual problem in the science and technology. Such studies are of great importance for the rise in the effectiveness of the metallurgical manufacture, in particular, the electrolytic refining of copper and other metals. Besides, modelling of electric fields allowed to study electric and magnetic fluxes, and also the streams of the charged particles (a dust, gases), which is useful in the design of the industrial filters, and systems of pipeline airing of the deep open-cast mines.

The transfer of substance in the course of the electrolytic refining is carried out by three mechanisms: the molecular diffusion, the migration and the convection. According to this the streams of the diffusion, migration and convection are considered. The total stream involves all of these streams [6].

This paper is devoted to the modeling of the migratory ions stream in the electrostatic field of electrodes as applied to the electrolytic refining and the gas purification.

The algorithms collectively known as "methods of particles"[7]–[9] find increasing applications in the current mathematical modeling. The distinctive feature of these methods is the special mode of discretization wherein the set of discrete objects or the model particles is introduced as a grid of the mobile points. The methods of particles are applied to the problems where the evolution of some medium in a time or the result of such evolution is investigated (see, for example, [4], [7]–[9] and references therein). Initially the methods of particles were gotten the greatest development in the fields of applied research where the wide intellectual and computing resources were concentrated for the large-scale computing experiments. As examples works in the fields of the computing physics of plasma [3], gas dynamics [1]–[2], [7]–[9] and other areas [3,6] can serve as examples of such areas of study.

Among the methods of particles the purely Lagrangian and mixed algorithms are distinguished. The algorithms of the first group are reduced to a numerical integration of dynamic systems of differential equations [4] which describe the trajectories of the interacting particles. The mixed algorithms are characterized by that the evolution of the particle system is modeled in two steps on each temporal interval. In one of the steps, under the fix position of the particles the result of their interaction and (or) collective action on a medium is calculated. The calculation are carried out on a stationary ("Euler") grid. Therefore this step is called as the Euler stage. Another step, called the Lagrange stage, consists of solving the dynamic system on the next temporal interval provided that the right term of this system was calculated at the Euler stage.

The methods of particles, as a rule, are characterized by rather poor precision. Usually the relative error is as much as few percents. This resulted from the established compromise between the reasonable volume of computations and the possibility to model complicated phenomena. Such approach effects an essential economy of the machine time.

Unlike the problems of physics solving by the methods of particles where the processes run with the high velocity in a short time, the above technological processes are slowly current and takes much time. This determines the choice of the methods of particles-in-meshes for modeling of the technological processes because they feature a large supply of stability and allows for rather fast proceeding through an evolutionary variable. However the methods of calculation of the field potential used in the works mentioned above (for instance, the method of the fast Fourier transformation) are not suitable for the technological processes because of the essential error accumulation with time.

The paper is organized as follows. Section 2 is devoted to the mathematical model of the stream of the ions. The mixed method of particles is adapted for modeling of the migratory diffusion of a stream of ions in the course of electrolytic refining. At the Eulerian stage potentials of an electrostatic field are modelled by means of Maxwell's equations. At the Lagrangian stage the motion laws and the trajectories of ions are modeled in the form of the square-law splines. In Section 3 the results of the computer modelling of the ions stream are discussed.

2 Mathematical model of the ions stream

As a basic mathematical model of driving the charged particle we take the laws of driving of an ion under the electric force. It is supposed that particles are distributed uniformly at the plane anode. For every portion of a trajectory the separate equations of driving ions are constructed which allows to find the coordinates and the velocity of a particle at any moment t. We consider driving in the normal direction to the surface of electrodes. The real trajectory of driving is casual because the velocity and the acceleration of the charged particle at each point of the trajectories depends on casual collisions with other charged particles or a wall of the dielectric capacity. Therefore the vector of acceleration defined by the electric field strength is found and used for calculation of a velocity at each point.

The strength of the electrostatic field is defined as an antigradient of a potential f of a field (see [7])

$$\mathbf{E} = -\mathrm{grad} f.$$

In accordance with Maxwell's equations

$$-\mathrm{div}\mathbf{E} = \mathrm{div}\,\mathrm{grad} f \equiv \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0. \quad (1)$$

Hence the potential f satisfies the Laplace equation in the domain $D = \{x \in (-d/2, d/2), y \in (0, l_1)\}$ and the boundary conditions

$$f(-d/2, y) = q, \quad f(d/2, y) = q_A, \quad f(x, 0) = f(x, l_1) = 0 \quad (2)$$

where q_A – the charge at the anode.

Let the particle reach the second electrode over the period T, i. e. t ranges from 0 to T. We consider so small time interval Δt that the strength $\overline{E} = (E_x, E_y)$ can be taken as being approximately constant on a portion of the particle trajectory from the point $(x(t), y(t))$ to the point $(x(t+\Delta t), y(t+\Delta t))$. Then the model of the motion law for the charged particle can be represented in the form of a vector function $\overline{S} = (S_x(t), S_y(t))$ where $S_x(t)$ and $S_y(t)$ are the square splines constructed on the grid: $\omega : t_i = i\Delta t$, $i = 1, 2, \ldots, n$, $n = T/\Delta t$. On every segment $[t_i, t_{i+1}]$ the vector $\overline{S}$ is defined by functions [7]

$$S_x^i(t) = \frac{qE_{xi}}{m}\frac{(t-t_i)^2}{2} + v_{xi}(t-t_i) + S_x^{i-1}(t_i), \tag{3}$$

$$S_y^i(t) = \frac{qE_{yi}}{m}\frac{(t-t_i)^2}{2} + v_{yi}(t-t_i) + S_y^{i-1}(t_i). \tag{4}$$

where

$$E_{xi} \equiv E_x(S_x^{i-1}(t_i), S_y^{i-1}(t_i)),$$

$$E_{yi} \equiv E_y(S_x^{i-1}(t_i), S_y^{i-1}(t_i)).$$

In the case of a collision between two particles flying with the velocities $\bar{v}_1(t^*)$ and $\bar{v}_2(t^*)$ at the moment $t^* \in [t_i, t_{i+1}]$ the trajectory of the first particle changed with respect to the following law:

$$S_{1x}^i(t) = \begin{cases} \frac{qE_{xi}}{m}\frac{(t-t_i)^2}{2} + v_{1x}^i(t-t_i) + S_{1x}^{i-1}(t_i), & t_i \le t \le t^*, \\ \frac{qE_{xi}}{m}\frac{(t-t^*)^2}{2} + v_{1x}^i(t-t^*) + \frac{qE_{xi}}{m}\frac{(t^*-t_i)^2}{2} & \\ +v_{1x}^i(t^*-t_i) + S_{1x}^{i-1}(t_i), & t^* \le t \le t_{i+1}; \end{cases} \tag{5}$$

$$S_{1y}^i(t) = \begin{cases} \frac{qE_{yi}}{m}\frac{(t-t_i)^2}{2} + v_{1y}^i(t-t_i) + S_{1y}^{i-1}(t_i), & t_i \le t \le t^*, \\ \frac{qE_{yi}}{m}\frac{(t-t^*)^2}{2} + v_{1y}^i(t-t^*) + \frac{qE_{yi}}{m}\frac{(t^*-t_i)^2}{2} & \\ +v_{1y}^i(t^*-t_i) + S_{1y}^{i-1}(t_i), & t^* \le t \le t_{i+1}; \end{cases} \tag{6}$$

In a similar manner, the trajectory of a second particle is changed by the law

$$S_{2x}^i(t) = \begin{cases} \frac{qE_{xi}}{m}\frac{(t-t_i)^2}{2} + v_{2x}^i(t-t_i) + S_{2x}^{i-1}(t_i), & t_i \le t \le t^*, \\ \frac{qE_{xi}}{m}\frac{(t-t^*)^2}{2} + v_{2x}^i(t-t^*) + \frac{qE_{xi}}{m}\frac{(t^*-t_i)^2}{2} & \\ +v_{2x}^i(t^*-t_i) + S_{2x}^{i-1}(t_i), & t^* \le t \le t_{i+1}; \end{cases} \tag{7}$$

$$S_{2y}^i(t) = \begin{cases} \frac{qE_{yi}}{m}\frac{(t-t_i)^2}{2} + v_{2y}^i(t-t_i) + S_{2y}^{i-1}(t_i), & t_i \le t \le t^*, \\ \frac{qE_{yi}}{m}\frac{(t-t^*)^2}{2} + v_{2y}^i(t-t^*) + \frac{qE_{yi}}{m}\frac{(t^*-t_i)^2}{2} & \\ +v_{2y}^i(t^*-t_i) + S_{2y}^{i-1}(t_i)(t_i), & t^* \le t \le t_{i+1}. \end{cases} \tag{8}$$

When striking the bottom of the electrolytic bath the angle of incidence of the particle is equal to the angle of reflection from the bottom. In this case the trajectory of a particle is modeled as follows:

$$S_x^i(t) = \begin{cases} \frac{qE_{xi}}{m}\frac{(t-t_i)^2}{2} + v_x^i(t-t_i) + S_x^{i-1}(t_i), & t_i \le t \le t^*, \\ \frac{qE_{xi}}{m}\frac{(t-t^*)^2}{2} - v_x^i(t-t^*) + \frac{qE_{xi}}{m}\frac{(t^*-t_i)^2}{2} & \\ +v_x^i(t^*-t_i) + S_x^{i-1}(t_i), & t^* \le t \le t_{i+1}; \end{cases} \tag{9}$$

$$S_y^i(t) = \begin{cases} \frac{qE_{yi}}{m}\frac{(t-t_i)^2}{2} + v_y^i(t-t_i) + S_y^{i-1}(t_i), & t_i \le t \le t^*, \\ \frac{qE_{yi}}{m}\frac{(t-t^*)^2}{2} + v_y^i(t-t^*) + \frac{qE_{yi}}{m}\frac{(t^*-t_i)^2}{2} & \\ +v_y^i(t^*-t_i) + S_y^{i-1}(t_i), & t^* \le t \le t_{i+1}. \end{cases} \tag{10}$$

In all of the described situations the coordinate z is constant, that is z = z0.

The above model could be used for modeling of the streams of both cations of metal and anions of acid residual. Unlike cations of metal, anions of acid residual migrate freely in the electrolytic bath without the deposition at the electrodes.

3 The computer modeling of a stream of charged particles

The ions of copper are the charged particles of the same type and had the same mass. The mass of such particles is taken to be equal to 1 for all particles. In the initial moment the charged particle resides at a point $(0, y_0, z_0)$. The trajectories of particles are formed by laws (3)–(10) with $m = 1$.

In the electrolysis bath electrodes are parallel to each other. At such disposition of electrodes of $v_{0x} = 0$. Initial coordinates y_0, z_0 of the charged particle is modeled by the Monte-Carlo method as random variables obeys the uniform distribution law. In view of the kinematic equations (6), (7) of the plane motion the first portion of a spline is defined by the formulae (3), (4) for $i = 1$ under the constant strength of an electrostatic field.

Further, the coordinates of the particle (x_1, y_1, z_0) at the moment $t = t_1$ and the average velocity of the transfer of the particle to the point with these coordinates is modeled by means of (3)–(10). The process proceeds until the particle reaches the boundary of the area of modeling. When the particle reaches the lower horizontal boundary of area, the impact of the particle with a bottom of capacity is modeled. If the coordinates of two various particles are coincided at some moment of time, the collision of particles is modeled. In case of nce of the coordinates of a particle are coincident with the coordinates of a point at the cathode, then the deposition takes place.

The area of modelning represents the electrolyte-filled space between the alternating cathodes and anodes. The space is surrounded are by the dielectric walls and bottom of the bath. The area is parallelepiped in form.

The charge on electrodes is taken to be uniformly distributed, as well as in [7]–[9]. The potentials of electrodes does not depend on their width z and are modeled in the plane of coordinates and y. For the five-point difference scheme is used for calculation of the potential from the problem (1), (2). The difference scheme is constructed on a grid with the same mesh width h with respect to x and y.

The mathematical model of a stream of particles (1) - (10) can be applied to modelling of gas purification and airing with the only difference that the mass of the charged particles can vary. The computer experiments on modeling of gas purification were pursued for the electrofilter EGAV 1-40-9-6-4 used at Open Company "Krasnoyarsk cement"for refining of depart gases.

4 Conclusion

The proposed algorithm allows to apply the method of particles-in-meshes to modeling a stream of ions between the anode and the cathode is created at electrolytic refinement. The method is applied to modelling of streams of ions of metal and acid residual in the laboratory equipment for. The numerical and computer experiments on were made for modeling the streams of the charged particles in the electrolytic copper refining and gas purification.

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