

Mathematical Simulation of Crystal Growing in Water-Salt Solutions

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Abstract—A detection of the conditions of high-rate single crystal growth with an appropriate quality is a priority for an industrial production of crystalline materials. The crystals of potassium dihydrogen phosphate (KDP) are the important optical materials. They are growing from water-salt solutions. The flow and mass transfer are modeled within the framework of continuous medium, which is considered as a water solution of a special salt-potassium dihydrogen phosphate. This salt dissolves in water to a saturation level at a high temperature. Then, such supersaturated solution is used to grow crystals at lower temperatures in static crystallizers (without inflow and outflow) and in continuous-flow crystallizers. The mathematical model is considered in a conjugate formulation with taking into an account of mass transfer in “solution–crystal” system. The local features of hydrodynamics and mass transfer in a solution near a surface of growing crystal are established, which may affect to a local (for a particular place and direction) crystal growth rates and a defect formation. The requirements to the crystallizers for providing a “necessary” solution hydrodynamics are discussed. The validation of this model is shown for the task of flow around a long horizontal plate, which simulating the growing crystal facet. The rate of salt precipitation is estimated by means of proposed mathematical model, in which a solution flow and salt concentration are calculated by solving Navier-Stokes and mass transfer equations for an incompressible fluid. Then the calculated salt flux on crystal surface is applied in a thermodynamic relationship for a normal growth of facets under conditions of two-dimensional nucleation. The action of continuous-flow crystallizers was analyzed for various solution inflows (axial and ring) and its outflow through the bottom hole.

Keywords: computer simulation, mass transfer, impurities, interfaces, saturation

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1. INTRODUCTION

May be the two possible mechanisms of layer-by-layer growth of crystals: dislocation-spiral and two-dimensional nucleation. At the high supersaturation of solution, the conditions for realizing the mechanism of two-dimensional nucleation are created [1].

In this case, the growth sources are two-dimensional nuclei formed over the entire crystal surface. The first time at super-high supersaturations 0.55 – 0.6, KDP crystals with linear dimensions ~10 mm were grown [2].

Steady reproduction of such crystal growth causes the development of new devices and technological regimes for high-speed growth of KDP crystals. This is connected with the formulation and solving little studied or essentially new problems of hydrodynamics and mass transfer in water-salt solutions characterized by the three-dimensionality of a container, the channels of solution inflow and outflow, the complex geometry and location of a crystal in a solution volume, by the presence of rotating or vibrating devices for intensifying mixing [3–5], etc.

Convection in solution may both increase a growth rate and enhance a morphological instability of crystal growth surface, which may worsen a crystal quality. From an experimental study [6] follows: the convection may lead to an inclusion formation. However, in other work it was noted that the convection leads to a weakening an inclusions formation [7] and assists to an increase of a growth rate without corrupting a crystal quality [8].

A number of experimental [9–12] and theoretical [13, 14] studies were carried out to determine a convective influence on the morphological growth instability and inclusions formation. It was shown that the solution flow direction near the solution/crystal boundary significantly influences on an appearance of morphological growth instability. If a flow is directed against a movement of growth steps, the morphological growth stability is preserved. On the contrary, the solution flow along the steps direction leads to a morphological instability.

The study [15] has showed that a morphological stability may be significantly enhanced by creating the reverse flows. However, the reversible flows creating by means of a reversibly rotating crystal do not cover the entire crystal surface. Therefore, a large area of crystal surface remains as morphologically unstable and the problem of inclusions formation remains, too. The supersaturation distribution of a growth surface depends on the direction and rate of solution flows. This value plays a significant role in an emergence and development of morphological instability, as well as in inclusions formation.

It was shown in [16] that the crystal rotation rate affects to a surface supersaturation distribution and a magnitude of “stepwise bend” and, as a consequence, this determines a morphological stability of crystal growth and inclusions formation. It was shown in [17] that a change in the flow characteristics near the crystal surface by adjusting its orientation may eliminate the regions of low supersaturation on crystal surface and limit the inclusions formation. It is assumed that there is a relationship between the distribution of surface supersaturation and inclusions formation. Therefore, in known experiments the location of a region having the low supersaturation corresponds to a region with inclusions.

The flow and mass transfer in solution systems determine supersaturation on the crystalline surface. However, an experimental determination of the surface saturation distribution is difficult. Therefore, it is important numerical simulation of a flow and mass transfer taking into an account of a crystal growth from the solutions. Such work has been carried out in [18], where three-dimensional and time-dependent flows have been studied for KDP crystal growth and their essential effect on crystal growth was shown. In [19], a two-dimensional simulation of the combined effect of forced and natural convection on KDP crystal growth has been carried out, which has showed that for a suppression of natural convection, a significant intensity of a forced flow in the crystallization chamber is required.

Three-dimensional and time-dependent calculations of turbulent flows have been carried out in [20], which taking into an account of the conditions of a high-rate KDP crystal growth. These calculations have been showed that the flow dynamics and a supersaturation distribution strongly depend on the crystal size, the growth rate, and the crystal rotation rate. The “self-consistent” model for KDP crystal growth was proposed in [21], in which both the bulk diffusion and the reaction on a crystal growth surface were taken into an account for a determination of the diffusion layer thickness around a crystal.

The mathematical model of crystal growth must be considered in a conjugate formulation with taking into an account of a mass transfer in “solution-crystal” system. It is necessary to establish the local features of hydrodynamics and mass transfer in a solution near a growing crystal, which may affect to a local (for a particular place and direction) crystal growth rate and a defect formation. Unfortunately, at the present time the number and variety of different devices for providing “needful” solution hydrodynamics significantly exceeds the number of studies of hydrodynamics and mass transfer in such devices.

In this paper, a mathematical model of flow and mass transfer is proposed to describe the process of salt crystallization from a solution. Its approbation was considered for the problem of crystallization on a streamlined horizontal plate. The calculation model analyzes the solution hydrodynamics in crystallizers intended for KDP crystal growth. The features of hydrodynamics and mass transfer on a crystal surface are revealed with taking into an account of technological conditions [2] and the criteria for ensuring two-dimensional nucleation [1]. For mathematical modeling the software [22] was used.

2. MATHEMATICAL MODEL OF FLOW AND MASS TRANSFER FOR CRYSTAL GROWTH FROM SOLUTION

The flow and mass transfer are studied within the framework of continuous medium modeling, which is considered as a water-salt solution of KDP. This salt dissolves in water to a saturation level at a high temperature. Then, such a supersaturated solution is used in crystal growth at lower temperatures in static crystallizers (without inflow and outflow) and in continuous-flow crystallizers.

In the static crystallizers, the salt-saturated solution is cooled, creating conditions of salt precipitation (crystallization) on seed crystal, and in the continuous-flow crystallizers a solution is continuously pumped at given temperature and corresponding supersaturation level. One of the variants of the continuous-flow axisymmetric crystallizer is shown in Fig. 1. It is characterized by axial inflow and outflow of solution in the directions indicated by arrows.

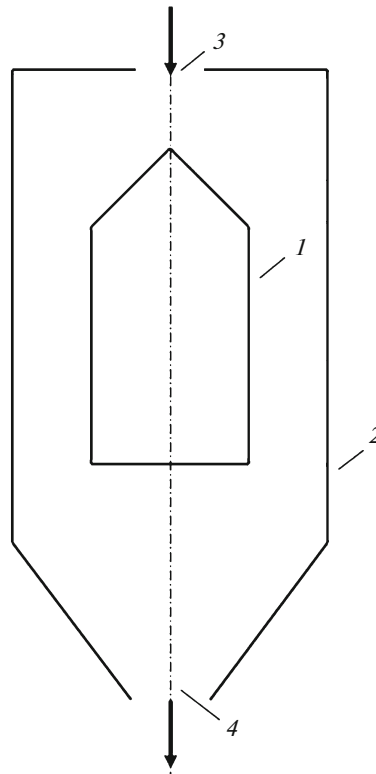


Fig.1. Scheme of the crystallizer with axial inflow and outflow of solution: (1) – growing crystal, (2) – crystallizer body, (3, 4) – holes for inflow and outflow of solution in the directions shown by arrows.

The working temperature of KDP solution in the crystallizer was maintained at 32°C, and the salt saturation was made at a higher temperature (69°C) to a concentration $C_o = 1.59503 \times 10^{21}$ molecules per 1 cm³ of solution.

For the operating temperature $T = 32^\circ\text{C}$ an equilibrium salt concentration is $C_e = 9.98578 \times 10^{20}$ molecules per 1 cm³ of solution. It is possible an estimation of the supersaturation at $T = 32^\circ$ by means of the following formula:

$$\sigma = \ln(C_o/C_e) \quad (2.1)$$

and its value in a particular case is 0.47.

From the point of view of mass transfer, the salt precipitation occurs in a solution volume, on a seed crystal and walls of crystallizer. The presence of crystalline nuclei in solution causes their volumetric expansion according to thermodynamic laws, which can be considered in conjunction with the model of a fluid continuous medium.

To determine the velocity vector $\mathbf{V} = (V_x, V_y)$ and the pressure P in the solution, the Navier-Stokes equations for an incompressible fluid are solved. They are written in vector form as follows:

$$\partial \mathbf{V} / \partial t + (\mathbf{V} \nabla) \mathbf{V} = -1/\rho \nabla P + \nu \Delta \mathbf{V}, \quad \text{div} \mathbf{V} = 0 \quad (2.2)$$

and together with (2.2) the equation of convective salt transfer is solved:

$$\partial C / \partial t + (\mathbf{V} \nabla) C = D \Delta C. \quad (2.3)$$

The salt concentration C is normalized to the inflowing C_o value and further it is considered in dimensionless form. Here: t is the time, ρ —solution density, ν —kinematic viscosity, and D —salt diffusion coefficient.

At the inflow boundary: the flow rate and salt concentration are set: $\mathbf{V} = \mathbf{V}_o$, $C = 1$. At the outflow boundary: the normal gradient of velocity and salt flux are equal to 0. And “non-slip” condition and the absence of salt flux are set on crystallizer walls.

Table 1. Parameters for calculating the crystallization rate of a facet

Parameter	Value
w —volume of the molecule, cm^3	9.68×10^{-23}
k —Boltzmann constant, erg/K	1.38×10^{-16}
β —kinetic coefficient, cm/s (32°C)	0.00955
α —specific energy of the step for the face (100), erg/cm^2	19.5
h —height of the step on the facet (100), cm	7×10^{-8}
D —coefficient of salt diffusion, cm^2/s (32°C)	7.5×10^{-6}
$\eta = \nu \times \rho$ —dynamic viscosity of solution, g/cm s (32°C)	1.5×10^{-2}

On crystallization front (crystal surface): the condition of “non-slip” on the flow and the condition of “mass flux” at rate R are applied:

$$D\partial C/\partial n = RC(k_0 - 1). \quad (2.4)$$

Here, in the balance of salt fluxes a diffusion flux with a coefficient D and a convective flux are taken into an account. They include a solution salt transfer and a flux into crystal with a normal velocity R .

In the boundary condition for a salt concentration (2.4) we use the parameter k_o , which is given for the solution-crystal surface by the ratio of the solidifying concentration — C_{solid} to the influx salt concentration from the solution volume — C_{liquid} : $k_o = C_{\text{solid}}/C$. May be note an analogue with a crystallization from a melt, where k_o is used as the equilibrium impurity distribution coefficient in the “crystal-melt” system [23].

In both cases, k_o is a certain phenomenological parameter, which quantitatively characterizes the impurity (salt) flows in a macromodel of the convective mass transfer during crystallization (from a melt or solution). However, if for a melt crystallization the parameter k_o is widely used in technological practice and experimentally measured for a large number of materials and impurities, then for the crystallization from the solution there are no approved approaches to its assignment.

In this paper, this parameter was used as the ratio of an equilibrium concentration C_e to a solution concentration at the end of concentration boundary layer C_δ , which for the given flow geometry was equal to inflowing concentration C_o , then $k_o = C_e/C_o$. Taking into an account of formula (1), this analogue has the equivalent notation: $k_o = e^{-\sigma}$, where $k_o \leq 1$.

It can be noted that in the limiting case, when there is no supersaturation of the solution with salt (for $\sigma \rightarrow 0$), there is no mass exchange of a solution with a crystal surface. Preliminary calculations were made to evaluate an applicability of formula (4), when the supersaturation was too high (at $\sigma \rightarrow 0.75$). At a low inflow rate (5 cm/s), a salt precipitation occurred intensively only near the solution inflow boundary. Then the solution concentration quickly became less than equilibrium and it meant that there was absent further crystallization downstream.

The parameter R , which in the theory of mass transfer means the rate of precipitation of a salt on a certain surface, in this case plays a key role in conjugating the hydrodynamic macro model with a micromodel describing the process of crystal growth. The parameter R is given in the form of a thermodynamic relation that takes into an account of a solution saturation level σ at a given temperature T and the parameters corresponding to the growth of the specific crystal face: β is the kinetic coefficient of the step, w is the volume of the particle in the crystal, h is the height of the elementary step, α is the specific surface energy of the step; here k is the Boltzmann constant. This relation is written in the form of the following formula [2]:

$$R = \beta\sigma^{5/6} \exp(-\pi w\alpha^2 h/2k^2 T^2 \sigma). \quad (2.5)$$

In this formulation, the specificity of the material is taken into an account of the equilibrium C_e concentration for the parameter k_o and in the parameters for R entering into for which the meanings and values are given in Table 1.

Analogously to [18, 20, 24], the crystallization rate R is given by a constant value for the given parameters from the Table and the supersaturation value $\sigma = \ln(C_o/C_e)$, and the mass transfer process is taken into an account in the boundary condition (2.4). Such model is useful for estimating the influence of



Fig. 2. The hydrodynamic boundary layer near horizontal plate at an initial velocity of the inflow $V_{xo} = 5$ cm/s: velocity isolines and vertical scale of V_x on initial plate part $x \leq 1$ cm.

hydrodynamic parameters on mass-exchange processes on the crystal surface. Its application will be considered in a simplified example below.

3. APPROBATION OF THE CONJUGATED MODEL ON THE FLOW AROUND A LONG HORIZONTAL FACET

We suppose that the creation of a homogeneous salt flux from a solution to a crystal is the necessary condition for KDP crystal growth by a way of two-dimensional mechanism of nucleation [2]. Such homogeneous salt flux takes place for the flow around a long horizontal plate (crystalline facet ~ 10 cm). Moreover, for an infinite plate there is corresponding analytical solution [25]. Therefore, this vortex less flow was chosen for approbation of the mathematical model described above.

The problem is solved numerically in a two-dimensional region, which is long in x and narrow in y direction: $0 \leq x \leq 10$ cm, $0 \leq y \leq 0.5$ cm. The salt solution inflows parallelly to this plate through the cross-section $x = 0$ at the velocity V_x . The deceleration of this flow along the plate causes a change of the velocity profile, which corresponds to thickening of the hydrodynamic boundary layer in picture of isolines V_x (Fig. 2).

A flow deceleration along the plate causes a vertical salt flux inhomogeneity near a plate surface, which increases with a removal from the inflow cross-section. This may be seen from a comparison of the vertical profiles $C(y)$ concentration shown in Fig.3: for the beginning ($x = 1$ cm) and the end of the plate ($x = 9$ cm). Their comparison shows that at a supersaturation $\sigma = 0.47$, the salt concentration C on the plate surface decreases from 0.87 to 0.73. The result of this decrease should be as slowing down of crystalline facet growth at removal from inflow cross-section. The calculated profiles correspond to analytical estimates of the diffusion layer thickness $\delta = 500$ μ at inflow rate $V_{xo} = 5$ cm/s [25].

An applicability of proposed mass transfer model was investigated by analyzing the results of parametric modeling, which were obtained at various supersaturations $\sigma = 0.1 \div 0.7$ and at two rates: $V_{xo} = 5$ and 30 cm/s (Fig. 4), and at different rates $V_{xo} = 5 \div 30$ cm/s and one supersaturation $\sigma = 0.47$ (Fig. 5). In Fig.4 the equilibrium dimensionless concentration $C_e = 0.626$ at $T = 32^\circ\text{C}$ is indicated by the dash line.

An analysis of Fig.4 shows that at low supersaturations ($\sigma = 0.1 \div 0.3$) the salt concentration varies slightly along plate length (see $C_{x=9\text{ cm}} = 1 \div 0.95$), but at large supersaturations ($\sigma = 0.4 \div 0.7$) the significant concentration decrease toward a plate end is observed.

In the experiment mentioned at the beginning of this section, the working supersaturation was $\sigma = 0.47$, which corresponds to $C_{x=9\text{ cm}} = 0.73$ or in the dimensional form is 11.64372×10^{20} molecules per 1 cm³ of solution. This exceeds the equilibrium value $C_e = 9.98578 \times 10^{20}$ at $T = 32^\circ\text{C}$. In this case at such conditions a long facet may be grown.

However, for large supersaturations the insufficiently high inflow velocity ($V_{xo} = 5$ cm/s) leads to a significant concentration salt decrease at plate end to the values below an equilibrium level (see Fig. 4). This indicates that such long facet cannot grow under these conditions.

A possible way out of this situation may be an increase of solution rate V_{xo} . This conclusion follows from an analysis of graphs in Fig. 5. It may be seen that an increase V_{xo} from 5 to 30 cm/s substantially equalizes a concentration distribution along a plate length and significantly increases its values at plate end.

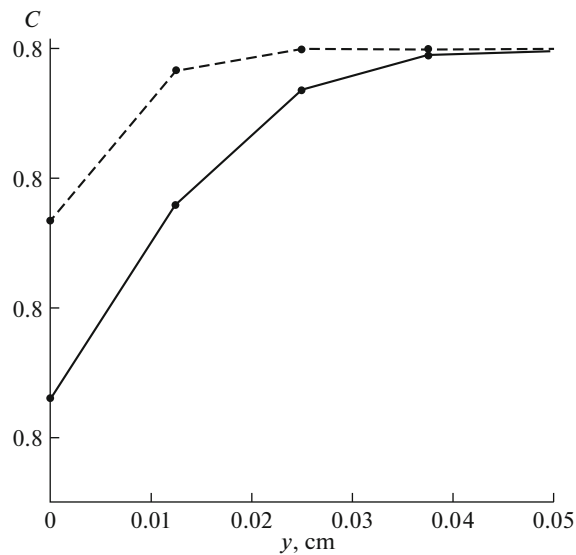


Fig. 3. The vertical distribution of salt concentration $C(y)$ for supersaturation $\sigma = 0.47$: at beginning ($x = 1$ cm)—dash line and at end of the plate ($x = 9$ cm)—solid one.

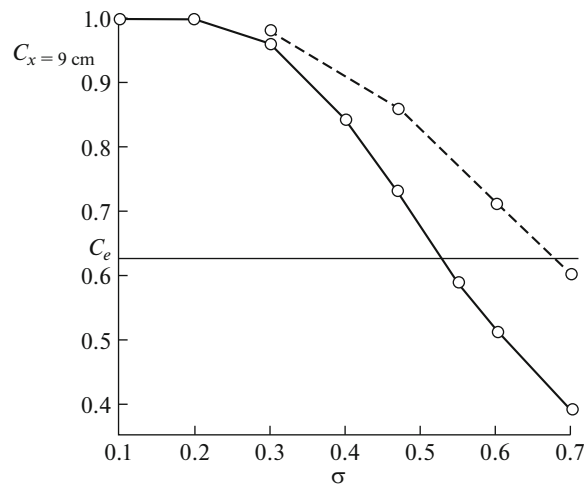


Fig. 4. The dependences of salt concentration $C_{x=9 \text{ cm}}$ at plate end ($x = 9$ cm) upon a supersaturation σ at two inflow rates V_{x0} (5 cm/s—solid line, 30 cm/s—dash line).

Thus, even for such vortex less flow around a sufficiently long facet, a coordinated optimization of a salt saturation and an inflow solution rate is required.

4. THE FLOW FEATURES IN CRYSTALLIZERS WITH AXIAL AND RING INFLOW OF A SOLUTION

In contradistinction to standard designs for crystal growth from a melt (for method of Czochralski [26] etc.) the various crystallizer designs are applicated for crystal growth from water-salt solutions, in which, according to the designers, the necessary crystal growth conditions are supported by means of best its flow-around (by velocity value and direction of flow, saline saturation solution and its temperature). In this article the hydromechanical problems are considered for continuous-flowing axisymmetric crystallizers.

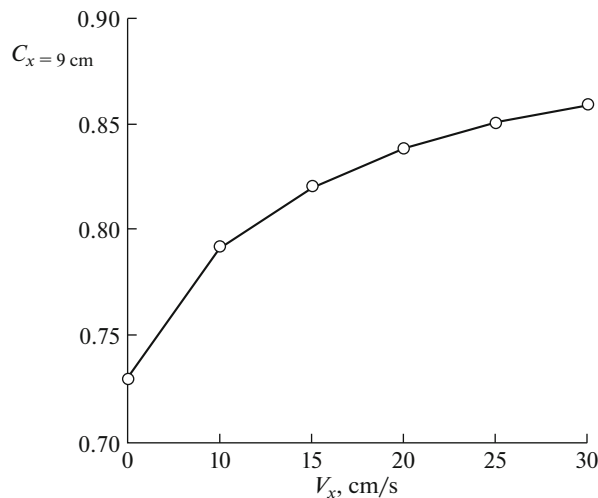


Fig. 5. The dependence of salt concentration $C_x = 9$ cm at plate end ($x = 9$ cm) upon a flow velocity V_{x0} at $\sigma = 0.47$.

The cases of axial and ring inflow of a solution are considered for which the crystal had a cylindrical shape with the following dimensions: the height of the conical part is 5 cm, the cylindrical part is 15 cm, and the diameter is 10 cm. Axisymmetric flows are realized for such crystallizers.

During an axial inflow of a solution and a static crystal, a lateral vortex flowing around a conical crystal part and a smaller vortex near its cylindrical part are formed (Fig. 6a). A formation of this small vortex, as well as a vortex under a crystal bottom, is explained by ledges in a crystal shape. These ledges create stagnant flow zones in which the conditions of convective mass transfer near crystal surface are different from the conditions on remained surface.

A crystal rotation leads to well-known hydrodynamic structure between two cylinders, characterized by a formation of a vortices chain along a cylindrical surface. This affects to an inhomogeneity of a salt transfer to the crystal surface from a solution volume (Fig. 6b).

For the case of solution inflow through top ring hole a non-vortex flow of a solution around a lateral crystal surface occurs (Fig. 7). This flow forms uniform conditions of salt precipitation on a crystal surface. Moreover, under a crystal bottom the vortices are formed due a crystal rotation, which contributes to a bottom flow uniformity. In general, this variant most fully corresponds to the plane-parallel flow and its realization could provide the required uniformity of salt fluxes on a crystal surface.

5. CONCLUSIONS

In this paper, it is considered that for KDP crystal growth by the two-dimensional mechanism of nucleation is the maintenance of a vortex less flow around a crystal surface. This forms a uniform salt flux from solution volume to the crystallization surface.

The rate of salt precipitation is estimated by the proposed mathematical model based on solving Navier-Stokes and salt transfer equations for incompressible fluid, which are conjugated with the thermodynamic model for a crystal growth according to two-dimensional nucleation.

The application of this conjugation to the problem of plane-parallel flow around a long plate have showed its satisfactory agreement with both theoretical estimates [25], and experimental values of crystal growth rates [2]. However, even for such vortex less flow around a sufficiently long facet, a coordinated optimization of a salt saturation and an inflow solution rate is required.

The various crystallizer designs are applicated for crystal growth from water-salt solutions, in which the necessary crystal growth conditions are supported by means of best its flow-around (by velocity value and direction of flow, saline saturation solution and its temperature). The action of continuous-flow crystallizers was analyzed for various solution inflow (the top axial and ring inflow) and outflow through the axial bottom hole. It may be note that the ring solution inflow may ensure the vortex less flow around a crystal surface. In the case of ring inflow, the plane-parallel flow around the lateral crystal surface forms a uniform salt flux into its surface. In the case of axial inflow, the vortex flows appear in the solution volume, which is non-acceptable for realization of the mechanism of two-dimensional nucleation.

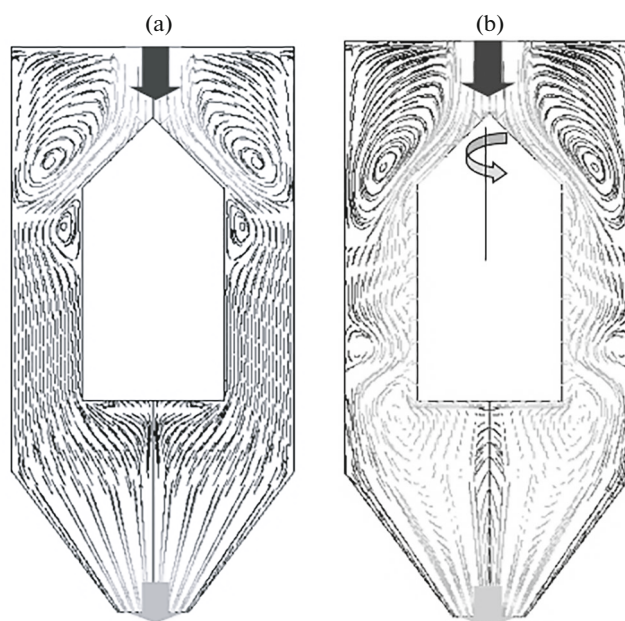


Fig. 6. The axial solution inflow into the crystallizer at rate 6 cm/s: a solution flow structure without rotating crystal (a) and with its rotation at angular rate 1 rad/s (b).

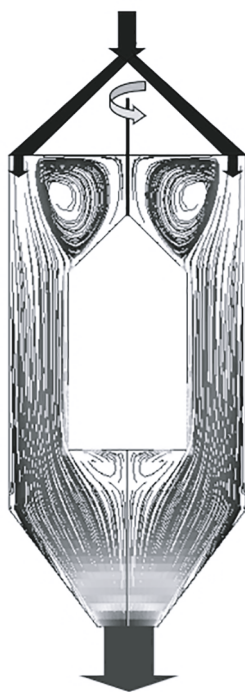


Fig. 7. The ring solution inflow into the crystallizer at the rate 6 cm/s: a solution flow structure with rotating crystal at angular rate 5 rad/s.

In comparison with the plane-parallel flow around a horizontal plate, considered in Section 3, the flows in real crystallizers are more complicated. For such problems, also possible application of conjugated mathematical model proposed in Section 2, although the corresponding calculations and analysis of their results will require much more necessary labor.

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