

# NUMERICAL MODELING OF MIXED CONVECTIVE FLOW AND MASS TRANSFER DURING THE HIGH RATE GROWTH OF AQUEOUS SOLUBLE CRYSTAL.

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Summary The hydrodynamics and mass transfer of KDP solution in a crystallization chamber are studied for non-stationary regime of feeding with different inflow boundary conditions. The numerical investigation of the flows and the concentration field above the growing crystal, based on the solution of 2D and 3D non-stationary Navier-Stokes equations in Boussinesq approximation and mass transfer equations is performed.

The high rate profiled monosectorial growth technologies (PMG) for aqueous soluble crystals have been developed due to the demand for large aperture nonlinear elements for power laser systems used in Inertial Confinement Fusion experiments. Profiled monosectorial crystal growth developed in the Institute of Applied Physics Russian Academy of Sciences (IAP RAS) is based on the growth in hard chambers with their cross section nearly equal to that of future elements. PMG enables to enhance the crystal growth rate 20 times as compared with traditional methods [1].

The main problems, arising while implementing this technology are connected with a morphological instability of growing crystal surface, caused by the interaction of growing surface with the rigid walls of the chamber, and organisation of material transport to the growing crystal.

An important feature of the PMG developed in the Institute of Applied Physics RAS is the intensive feeding of the solution near the growing crystal surface. Creation of a homogeneous concentration field in the boundary layer is one of the requirements imposed on the solution dynamics. Free convection leads to considerable inhomogeneity in the concentration field near the crystal surface. This inhomogeneity can be eliminated by optimizing the feed in order to suppress the natural convection. In the real experiment the intensive flow of a supersaturated KDP solution falls into the crystallization chamber through the oscillating multi-nozzle feeder which ensures a uniform feeding the growing crystal surface.

Therefore the study of flows above the crystal surface is very important for the understanding of fundamental mechanisms governing the interaction between natural and forced convection in crystallization chambers [2, 3]. New results of numerical simulation of the solution dynamics (free and forced convection) above the surface of a growing water-soluble crystal at varying inflow velocities are presented in this paper.

In order to find the optimal parameters providing the high-rate crystal growth without deterioration of the crystal quality, the numerical investigation of mixed convection in the crystallization chamber on the base of 2D and 3D non-stationary Navier-Stokes equations in Boussinesq approximation and mass transfer equation are performed. The efficient numerical scheme was developed and implemented for 3D non-stationary convection model. The Finite Volume method (FVM) discretization is applied to the regular staggered grid. Second-order discretization is used, with the quadratic upstream interpolation of advective terms (QUICK scheme). The time integration scheme is partially implicit, with the implicit treatment of the most critical terms. The pressure Poisson equation is solved by the novel highly efficient direct method that applies FFT in one direction, and employs 1-Way Dissection (1WD) method for solving remaining independent 2D elliptic equations. Using this new method instead of the traditional Fourier method (FFT + FFT + 3-diagonal solve) is necessary in order to apply a highly nonuniform grid in the vertical direction for the simulation of convective processes in very thin boundary layers near the surface of a growing crystal.

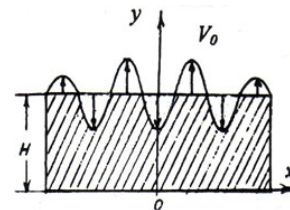
This numerical method is fully direct and doesn't involve costly iterative steps. The parallel version of this code exists, for performing simulations of time-consuming flows on supercomputers and clusters (using up to 16 processors) [4].

This numerical method is applicable to the simulation of unsteady spatial flows in laminar, transitional and turbulent regimes on fine grids for KDP crystal growth models. Here the models for cylindrical and rectangular domains are considered. The cylindrical coordinate system possesses some mathematical and numerical difficulties, and therefore it is important to obtain a method of validation and evaluation of different cylindrical codes.

A new benchmark is proposed in this paper as a tool for comparing cylindrical codes. The physical and mathematical formulations of this new benchmark are similar to those of previous benchmarks for 2D and 3D rectangular domains [5]. Benchmark results for three laminar regimes of natural convection are presented here for reference and comparison.

The simulations have shown that 2D approach is legitimate for the narrow rectangular enclosures used in KDP crystal growth setups in IAP.

The geometry of the problem is shown on Fig. 1. At the top of the crystallization chamber there are 3 inflow nozzles, each of the width  $2a$ . Chamber dimensions are  $H$  (height) by  $14a$  (width). Profiles of inflow and outflow velocity are shown for the stationary feeding. In this case, the flow can be modelled in half of region due to the symmetry. The boundary conditions for the velocity simulate the nonstationary inflow and outflow of the solution through the three-nozzle feeder. They are approximated by piece-wise parabolic profiles. The feeder oscillations are modeled by periodical shifting of the upper boundary. At the crystal-solution interface the constant gradient of the concentration is assumed, taking into account the real



**1. Geometry of the problem**

crystal rate growth at the corresponding parameters:  $c_y(x,0)=\text{const}=\alpha$ . This constant is determined using the hypothesis about a layer by layer growth without surface diffusion of adatoms and constant strength of growth centre.

The investigations were carried out for the following parameters of KDP solution:  $\nu=10^{-2}$  cm<sup>2</sup>/s,  $D=10^{-5}$  cm<sup>2</sup>/s,  $T_1 = 38^\circ$ ,  $T_2 = 41^\circ$ ,  $a=3.5$  cm,  $H=2$  cm, 5 cm and 10 cm, inflow velocities  $10$  cm/s  $< V_0 < 50$  cm/s for two different regimes of solution feeding: stationary inflow velocity, and periodical swinging of the upper boundary with the period  $T$ .

The calculations for stationary inflow velocity have shown that the regime of natural convection results in uncontrolled behaviour of the flow structure and concentration distribution in the boundary layer. When forced convection dominates over the solutal convection, we can control the flow structure and concentration field in the crystallization chamber. Moreover, forced convection ensures larger growth rate because the concentration boundary layer decreases.

The results for stationary inflow velocity show that the drop of the concentration in the crystallization boundary layer in two positions: just under the outflow nozzles (due to the excessive export of material from the crystal surface), and in the corners of the chamber (due to the wall friction, that decelerates the rising flow). Thus, in order to homogenize the solution near in the surface, an unsteady supply ensuring a periodic change in the regime of solution inflow and outflow near the surface of the crystal is organized.

As compared with the case of steady state flow, the concentration boundary layer inhomogeneities are significantly smoothed out. Migration of the depleted solution concentration peaks over the crystal surface during the period promotes homogenization of the time-average mass flow to the various parts of the surface of the growing crystal.

Numerical investigations show that with decrease of the feeder-crystal distance the homogeneity of the concentration boundary layer improves. Increasing the frequency of feeder oscillation leads also to homogenization of the concentration boundary layer.

The analysis of the flow structure and concentration field at different parameters (the supersaturating value, the value of the inflow velocity, the distance between the feeder and the crystal surface, and the frequency of the feeder oscillation) demonstrate the ability to control the concentration boundary layer in order to provide better homogenization needed for high quality KDP crystal growth.

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