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Selected laboratory benchmarks for validating numerical simulation of casting problems

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Abstract
The complicated physical phenomena which occur within solidifying metals during casting processes can not be easily observed. In the present paper the results of laboratory experiments with mould filling and freezing are presented. The experimental benchmarks have been constructed, based on so called *analog* fluids which are transparent and have well known physical properties: succinonitrile, polyethylene glycol, water and glycerine. The observed processes were investigated in small rectangular containers: inclined channel with forced flow, freezing at two isothermal, parallel walls; freezing from the top surface in a cubic cavity immersed in hot environment; volumetric freezing in a cube filled with fluid. Optical methods: Particle Image Velocimetry and Thermometry were applied for the flow analysis. Computer supported experimentation combined with digital data recording and processing allowed for the acquisition of a large amount of details on temporary temperature and velocity fields, as well as on phase front position. Herein the attention is focused on some technical problems illustrated by the examples of selected laboratory benchmarks for validating computer codes for casting problems.

1 Introduction

Due to industrial needs nowadays there is a common practice of applying complex computer analysis of new casting design. The computer codes used properly for modelling of flow and solidification processes provide valuable information, so the obtained results usually allow to reduce significantly the costs and time spent in the past on expensive trials. However, the numerical analysis implies introduction of several assumptions and simplifications of casting problems. The strong non-linearity of governing equations combined with a moving boundary make *a priori* prediction of consequences of inaccuracy or simplifications used in the numerical models almost impossible. This obviously appeals laboratory experiments to verify and validate numerical methodology used. Unfortunately most industrial problems involve configurations and substances which are very difficult to investigate experimentally.

Experiments used for computer code validation should reveal whether numerical results correctly describe physical processes, and if the process conditions and material properties can be taken into account properly. These fundamental questions can be answered having standard physical tests. The casting processes occurring in the real industrial environment are so complicated that still the required experimental data are not available and even there is no standard test for the specific certifications of numerical codes. The situation arises mainly from the fact that the metals have very high melting temperatures and still there is lack of the respective experimental technique for penetration and measuring specific quantities of the hot liquid interior.

Many research groups strive to establish the physical standard tests of casting processes and their achievements are regularly announced in the literature. The experiment presented by Sirrell and his coworkers on the Modeling of Casting conference constitutes one of the most important examples [1]. In fact, their results provided incomplete information on the liquid metal flow even though the expensive X-ray apparatus and temperature measuring system were used. This equipment allowed for the free-surface position recording, but still the solidification front, full velocity and temperature fields remained unknown. Thus, the qualitative agreement between experimental and numerical data could not be achieved. The alternative approach rely on the numerical codes validation using physical standard laboratory tests performed with so called *analog* fluids which are transparent, have well known physical properties and their melting temperatures are moderate.

The selected laboratory experiments, designed for validating numerical simulation of casting problems, are presented in the paper. They were obtained as a result of the laboratory analysis performed together with the respective numerical tests. Such procedure was utilized effectively in order to adjust the numerical models implemented in the computer codes to the real conditions and to better understand physics of the observed processes. The interaction between experiment and numerical analysis allowed to define the laboratory benchmarks for the mould filling process, solidification within filled container and coupling of filling and solidification.

2 Laboratory work stand designed for experimental benchmarks

The description of laboratory work stand used by the authors is presented in the sequel. The attention is focused on technical problems which arise when one strives to design experimental benchmarks for validating numerical simulations of casting problems.

2.1 Experimental methods

The measurements of velocity fields were done using the method known as *Particle Image Velocimetry* (PIV), where the flow field is visualized by the narrow thin sheet of light illuminating the tracers immersed in the moving liquid. The couples of consecutive registered and correlated images allow to determine the directions, magnitudes and orientations of velocity vectors in each point of the flow (Westerweel et. al. [2], Willert and Gharib [3]). The measurement accuracy can be increased when the correlation is replaced by optical flow method (Quénot et. al. [4]). This approach allows also to bypass specific inherent constraints of classical PIV method. In the present paper the analysis of hundreds of images had been done under Linux using a package of scripts control. The analysis included automatic filtration, proper texture formation, selected image part removal, vector fields calculations and results transformation to convenient graphical form.

The liquid temperature field was automatically measured using the method known as *Particle Image Thermometry* (PIT). The measurement is based on the fact that the light dispersed in the flow on the suspension composed of thermochromic liquid crystal (TCL) tracers changes its length depending on the liquid temperature and on the angle of illumination (Hiller and Kowalewski [5]). The procedure requires a calibrating curve of the variation of the most intensive light length with respect to the temperature which reveals the dominating color *Hue* (Kowalewski [6]). The relaxation time for typical crystals (50μm) is about 3 ms which is satisfactory for the analysis of thermal convection observed in the liquid. The measurement accuracy is *0.15K* for lower temperatures (colors varying between red-green) and *0.5K* for higher temperatures (blue colors).

Both experimental methods (velocity and temperature field measurements – PIV and PIT) were used by Hiller et. al. [7] for the thermal flow diagnosis and by Kowalewski and Cybulski [8] for the thermal flow coupled with phase transformation. In the present approach the same methods are used as a tool for collecting the data for validating numerical simulation of casting problems.

The experimental set-up recording flow images was composed of: convection container, camera, computer with image acquisition card, light source illuminating thin flow layer (1-2mm light-knife) in the observed process, resistance sensors used for local temperature registration (with accuracy ±*0.1K*), optical bench with the system of stepping motors and mirrors. The illuminated plane was observed by a CCD camera in the perpendicular direction. The positions of camera, light source and chamber could be changed using the system of stepping motors. The computer programs controlled: all movements performed by motors, light switching, collecting flow images, local temperature registration. Also all analysis of velocity and temperature field based on the registered hundreds of images in each experiment were performed automatically by "in house" computer codes.

2.2 Materials used in experiments

It has been decided that the polyethylene glycol ($H(OCH_2 CH_2)n OH$), succinonitrile ($NCCH_2 CH_2 CN$), glycerin ($C_3H_8O_3$) and distilled water were used as working analog fluids. The advantage of water is that its low viscosity allows to model the mould filling process with the high Reynold's numbers which are typical for casting problems. Two other materials, polyethylene glycol (in the sequel denoted as PEG 900) and succinonitrile, were chosen due to their phase transition character with the dendrite growth and over-cooling effects typical for metals. Both of them are often used as analog fluids for observations of solidification processes, so they are well described in the literature.

All flow and solidification processes were observed within the containers basically made from Plexiglass. This material was chosen because of its transparency, machining easiness and well known thermo-physical characteristic. The isothermal walls made of aluminum, copper, or Plexiglass (depending on the particular container design) were kept at constant temperature by flow of water or transparent polyethylene glycol, using thermostates.

Most of the material data used in numerical simulations were taken from the literature. The relations between kinematic viscosity and temperature for glycerin and glycol (PEG 900) were determined with the Heppler's viscosimeter.

2.3 Containers designed for experiments

The aim of laboratory procedure was to design experimental benchmarks for the processes characterized by interaction between the coupled phenomena: filling and liquid solidification. In fact, such coupling strongly depends on the selected geometry. The geometrical aspects become even more important taking into account that the optical methods (PIV and PIT) are used for the measurements.

In the simplest case, when the container is formed as a cube, the internal circulation deforms the shape of raising up free surface. When the forced flow vanishes the nonhomogeneous solidification is mainly caused by the natural and thermo-capillary convections, induced by the temperature gradients. As an essential effect of such thermal flows the complicated deformation of phase transformation fronts can be observed. These fronts together with the occurring at the beginning free surfaces constitute varying barriers for the light – it reflects and changes colors on them, so the measurement quality is deteriorated. The measurements are disturbed also when the container's transparency vanishes on the walls covered by solidifying material. The experimental difficulties are increased by the flow velocities varying within a wide range (the gradients can be extremely high) in each place where the containers have any corners, edges, etc.

Due to the above mentioned experimental problems the fundamental criterion for the choice of containers geometry was to confine the observed process complexity. Two simple shapes were used in the benchmarks described below, namely, the cube with upper isothermal wall (denoted as SIG) and the inclined rectangular prism with or without internal barriers (denoted as PBP or PZP, respectively).

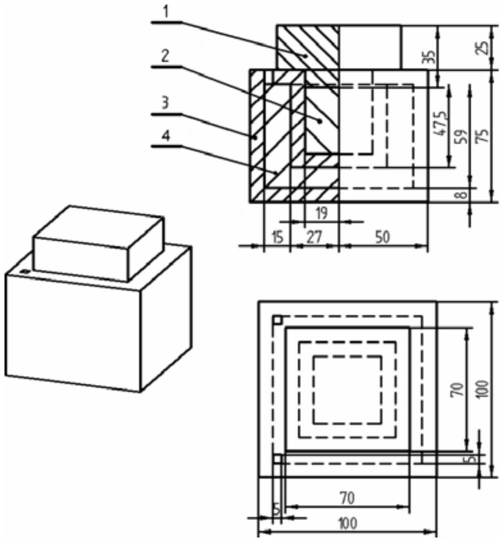

Figure 1: Scheme of cubic container (SIG) made of Plexiglas with cooling liquid layer: 1) aluminum plug, 2) chamber with analog fluid, 3) external wall, 4) external hot bath

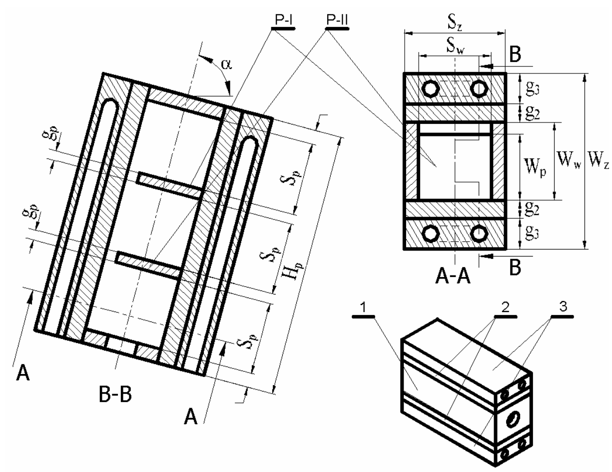

Figure 2: Scheme of rectangular channel (PZP): 1) walls made of Plexiglas, 2) and 3) metal covers with cooling channels; barriers P-I, P-II

Table 1: Dimensions of container PZP (and PBP without barriers; see Figure 2).

Variant	S_z	S_w	W_z	W_w	W_p	H_p	S_p	g_p	g_2	g_3
1	53	38	84	38	32.5	132	34.6	5	7	16
2	53	38	86	38	32.5	132	34.6	5	24	0

2.3.1 Cube with upper isothermal wall (SIG)

The idea which inspired the first laboratory benchmark of casting problems renders a Bridgman's set-up with a vessel containing the liquified precursor and the crystal product growing into the nutrient. The scheme of cubic container designed is presented in Figure 1. The aluminum plug (1) initiated a phase transition on the isothermal wall kept at the temperature T_c below the solidification temperature. The cubic cavity filled by the liquid (2) was immersed in the hot environment (4) where the flow confined by the external walls (3) had a controlled temperature T_{ext}. This design allows to control the heat flux transfer from the liquid to the surroundings. The thermal boundary conditions inducing natural convections and solidification in the cavity were determined by two temperatures T_c and T_{ext}.

2.3.2 Inclined rectangular prism (PBP/PZP)

The second container designed for laboratory benchmarks of casting problems is presented in Figure 2. The cavity dimensions and its inclination were modified during the experiments in order to get different regimes of the filling process. The basic variant PBP in the form of rectangular channel without internal barriers consisted of four walls made with Plexiglass and two other made with metal. The hot fluid was forced to the cavity through the circular opening placed in the bottom wall and its flow was illuminated through the upper wall. The course of flow inside the cavity was observed through the side walls (1). The metallic walls (2) with cooling channel (3) were assumed to be isothermal. The complexity of real mould was simulated by placing two plates inside the channel. The obtained variant PZP is partitioned into tree chambers connected by the narrow gaps.

3 Course of experiments

The data collected during the experiments comprise information on the velocity and temperature fields, and on the evolution of solidification fronts. Although the experiments were conducted in the simple cavities (cubic and rectangular prism), the processes observed were still quite complicated and the experimental results can be treated as challenging for validating numerical simulations. The list of presently discussed examples is given in Table 2. The first column comprises the original numbers used during the experiments. This numeration recalled in the sequel identifies the general problem characteristic defined in the consecutive columns, i.e.: problem type, geometry and material used, etc.

Table 2: List of experimentally analyzed problems

No.	Problem type	Geo-metry	Angle	Analog material	Boundary conditions		Initial conditions		Experimental details		
			α [°]		T_c [K]	T_{ext} [K]	v [ms^{-1}]	T_0 [K]	PIV	PIT	Tracers
#3	C	SIG	0.0	PEG-900	309.0	313.0	Cold start	313.0	●	○	glass spheres
#6	C+S	SIG	0.0	PEG-900	283.0	Ω	Ω	Ω	●	○	glass spheres
#18	C+S	SIG	0.0	PEG-900	302.0	313.0	Ω	311.0	●	●	TCL
							q ×10^6 [m^{3}s^{-1}]				
#40	F+C+S	PBP	11.4	Water	297.0	280.0	0.91	263.0	●	●	TCL
#47	F+C+S	PZP	82.0	Water	274.0	276.0	1.33	259.4	●	○	pine pollen

<u>Legend</u>
Problem type : F – filling, C – convection, S – solidification.
Symbols : Ω – set of values, ● – measurements done, ○ – measurements omitted.

3.1 Solidification in cube with upper isothermal wall (SIG)

The first presented benchmark was obtained as a result of two experiments, namely #3 and #6. When the stable convection within the cavity was achieved the thermostat controlling the temperature T_{ext} was switched of and the experiment #3 ended. The subsequent process rendered natural cooling and solidification within the mould. The appropriate measurements started and were performed during the experiment #6. Their aim was to investigate coupling between the natural convection and solidification influenced by the free thermal boundary conditions on the side walls of SIG container. The series of 5 flow images were registered in the central plane of the cavity in each 85ms interval. Then, they were correlated taking pairs collected in the different time intervals.

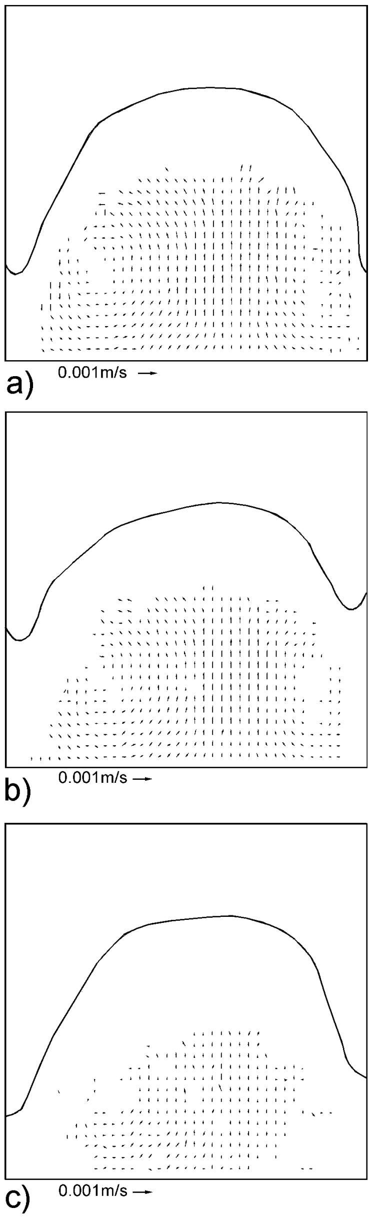

Figure 3: Velocity fields and phase transformation front evolution (Table 2, #6)

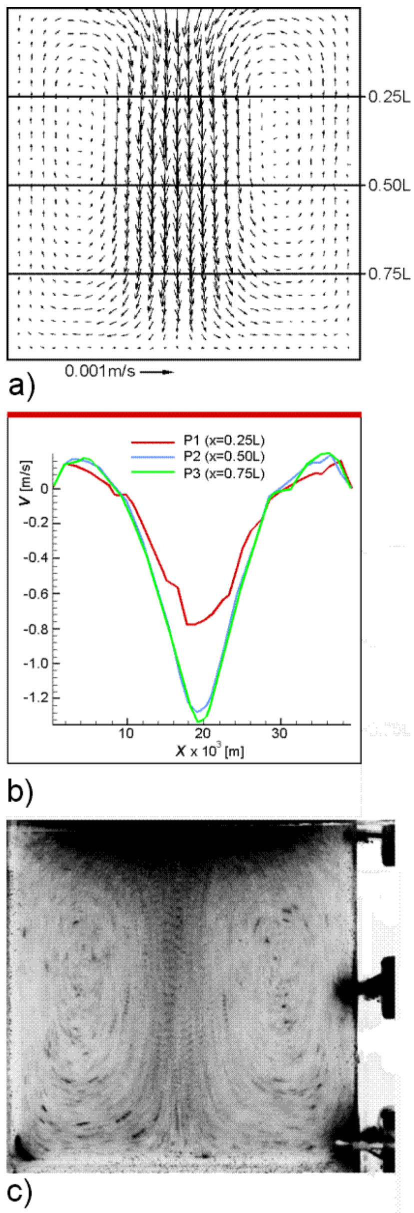

Figure 4: Velocity field (a), velocity profiles (b) and particle tracks (c) observed during stationary natural convection (Table 2, #18)

The thoroughly analyzed particle paths, temperature and velocity fields variation revealed the process sensitivity on the accuracy of cavity leveling. It was shown that the small imperfections can change significantly the direction of liquid flow and consequently the shape of phase transformation front. This important feature is illustrated in Figure 3. The experience gained during several trials resulted with a proper experimental methodology, so finally it was possible to obtain symmetric flow in the properly positioned container. The experimental results are treated as a benchmark for numerical simulation of velocity field. The characteristic feature of the process is that the solidification starts below the plug and then proceeds along the walls. The warm fluid is moving up along the axis of cavity symmetry and after cooling goes down along the side walls. The fluid is separated from the walls near the plug by a solidified material and the phase transition front becomes concave.

The shape of solidification front was different when the liquid surrounding the cavity in the experiment #18 was kept at the constant temperature T_{ext}. It was found in this case the solidified PEG-900 rendered a pyramid with four edges while the vertical components of flow velocities near the side walls were directed up (see [8]). The experimental results are treated as a benchmark for numerical simulation of the velocity field and the evolution of phase transition shape.

3.2 Coupled filling and solidification in rectangular prism

The preliminary experiments with the tilted channels were performed using succinonitrile, but the measurements were unsuccessful as the fluid forced to the cavity with the 343K temperature was quickly solidifying on the side walls decreasing their transparency. Such problem did not occur in the experiments described below where water had been used as an analog fluid.

3.2.1 Rectangular prism without barriers (PBP)

The water in the experiment #40 was forced through the inlet to the cavity with the flow rate *q* equal 0.91x10-6 m^3/s and the initial temperature equal 297K. The measurements started at the beginning of filling process and they were conducted by 974s. The registered flow velocity and temperature fields allow to assess the mutual influence of the mould filling and solidification process. The experimental results are treated as a benchmark for numerical simulation of the velocity and temperature fields and the evolution of phase transition boundary.

It seems that the most interesting result of that benchmark is that the flow velocities were very small at the end of the solidification process within the completely filled channel (see Figure 5a). It was observed that the flow structure was constantly varying, while the ice thickness was increasing slowly. The experimental data within that part of the process were collected at the cost of a reduced length of observed channel's view, but the registered images could have increased resolution. Consequently the improved measurement accuracy allowed to capture even small velocities and it is possible to create specific velocity profiles along selected paths. The examples of such profiles presented in Figures 5b and 5c correspond to the cross sections constructed along the lines P1 and P2 marked in Figure 5a. Computer simulation of such advanced stage of the solidification process seems to be challenging task, so the experimental data for validating numerical results can not be overestimated.

3.2.2 Rectangular prism with barriers (PZP)

The most important modification in the experiments #47 was that two lateral barriers were introduced into channel. These obstacles produced the additional light reflects. Different inclinations were tested in order to improve the measurements quality. The results presented in Figure 6 were obtained with the optimal angle α=82º. Once again the measurements started at the beginning of filling process and the coupling between water flow and solidification processes was observed. The initial temperature was established as 274K and the flow rate through the inlet was equal 1.33x10-6 m^3/s. The experimental results are treated as a benchmark for numerical simulation of the velocity fields and the evolution of phase transition shape.

The examples of registered results are presented in Figure 6. At the beginning water filling the first channel partition was cooled on the wall with the circular inlet. When the raising free surface reached the first barrier, then the subsequent flow down to the second partition resembled dam breaking problem. In both chambers two circulations formed quickly, but their directions were opposite.

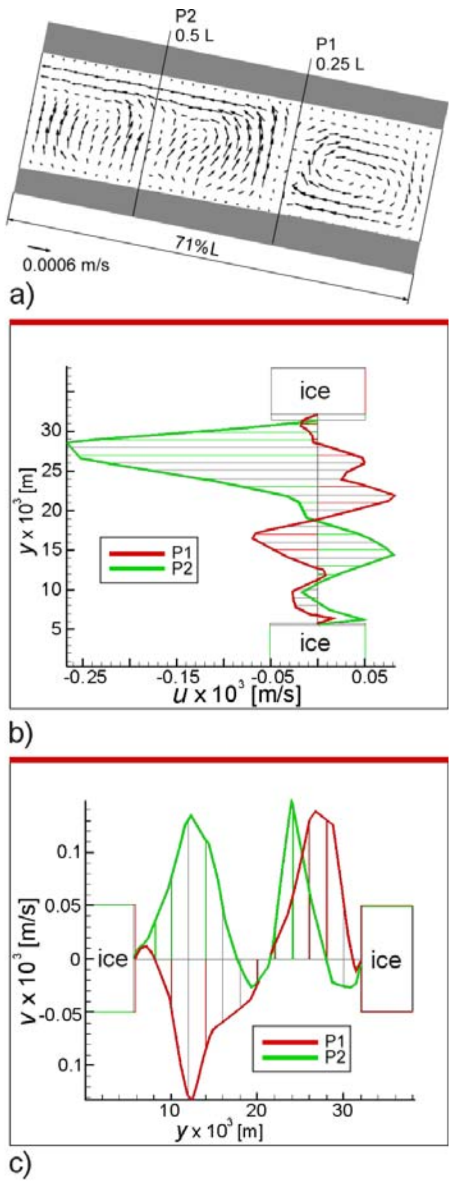

Figure 5: Measurements in freezing water – results registered after 974s: a) velocity field; b), c) velocity profiles (Table 2, #40)

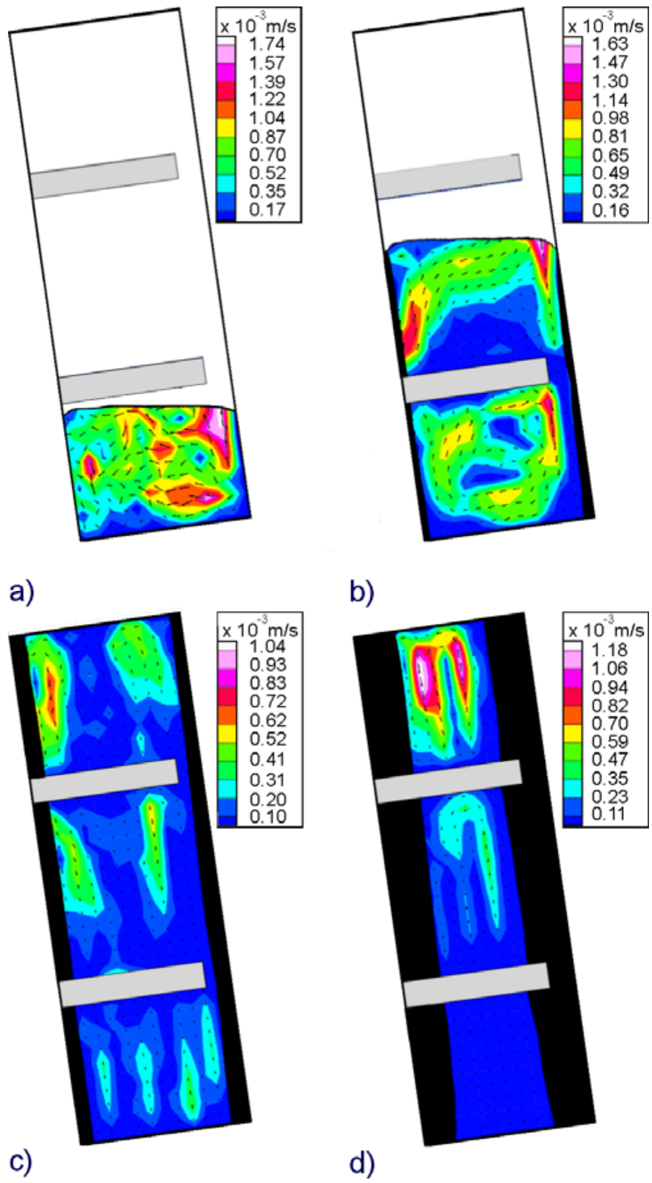

Figure 6: Evolution of velocity contours and ice volume growth in freezing water after:
a) 17s, b) 45s, c) 267s, d) 1163s (Table 2, #47)

It is worth to note that the clear waves along free surface in the vicinity of the second slit propagated contrary to the flow direction. When the second channel partition was completely filled subsequent recirculation became significantly slower and the main flow occurred at the top of cavity. The induced flow vanished when the whole container was filled. Further cooling and phase transition was controlled by the natural convection. Characteristic doubled vortices within the flow with recirculation were developing down along the walls and back through the cavity center. The flow across the slits became minimal and finally was completely blocked by the ice growing on the metallic walls.

4 Final remarks

The data obtained by the authors in series of experiments are available on the website and in several publications. The full set of results was presented in [9]. The collected information can be used as laboratory benchmarks which allow the validation of numerical models used in solidification problems.

The numerical tests performed by the authors with typical casting codes, some general purpose CFD codes, and available university codes indicated large sensitivity of the simulation results on thermal boundary conditions. Severe discrepancies were observed for data obtained with the casting codes. The performance and accuracy of typical approximation schemes: finite differences, finite volume and finite element method, were compared with a new mesh-free numerical approach, for a flow configuration typical for solidification problems. The finite volume method appeared favourable in accuracy whereas finite element in performance (speed). Performance and accuracy of the mesh-free approach was unsatisfactory. It indicates necessity for further development of its fundamental algorithms.

In general, casting codes should have their specific certification system. The laboratory benchmarks can significantly supplement typical technological methods used in the foundries. The optical methods (PIV and PIT) provide quantitative information on full velocity and thermal fields which are not available from industrial tests. Experiments together with mathematical models allow for proper interpretation of physical phenomena. The problem goes beyond the scope of the present paper. Herein the aim was to indicate the efficient tool for collecting experimental data useful for improving numerical algorithms.

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