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Simulations of Solidification in the Presence of Liquid Phase Movement

E. Gawronska, R. Dyja, N. Sczygiol

***Abstract*—The paper presents the results of the computer simulations of solidification with consideration of the liquid phase movement and dimensions of cast and mold. The problem of mass and the energy transfer is widespread in engineering, for instance, in designing ventilation systems or in founding. There is a multi-stage solution to the problem of convection in solidification simulations. The development of the numerical model with the momentum and continuity equations, and with conditions which are determined by the convection is a crucial tackle. Solving the Navier-Stokes (N-S) equations induces many numerical problems independently of the chosen discretization method. Moreover, numerical methods of solving the N-S equations are characterized by the significant time of calculations. Simulations were carried out with the use of our authorial software based on stabilized finite elements method (Petrov-Galerkin), which makes it possible to bypass the Ladyzhenskaya-Babuska-Brezzi (LBB) condition. In order to solve the N-S equation (with the convection element), Boussinesqs approximation was used. Finite Elements Method (FEM) was responsible for the description of the solidification process which is similar to the solution of the heat conduction equation (with the internal heat source responsible for the heat released during phase transformation). Convection causes movement in the liquid phase in the solidifying cast and can significantly influence the process of heat abstraction from the cast. It may change the distribution of the defects and the course of solidification during computer simulation, too. Integration over time has been done with the help of widely known one-step theta scheme.**

The computer simulations of solidification, which allow for the assessment of the influence of the cast size on the occurrence of convection and heat transfer, are presented. In order to find the solution, a computer implementation of the presented mathematical problems has been created. Results of this article make it possible to assess the cases in which the influence of the convection on the solidification process is significant. Based on the obtained results, it is feasible to state that the application of stabilization for FEM concerning the Navier-Stokes equations is an effective way to find the numerical solution regardless of the mold and cast dimensions. The authors of this paper intend to develop further the software to apply it to simulations connected with the problems in the foundry process.

***Index Terms*—numerical simulations, solidification, convection, Navier-Stokes, stabilized FEM**

I. Introduction

SOLIDIFICATION remains one of the most troublesome phenomena in numerical modeling. The number and variety of physical processes that take place between microscale and macroscale pose a significant dare to the scientists working on a suitable calculation model connected with diffusion and convection. The problem of mass transfer with energy transfer is quite prevalent thus the Navier-Stokes equations are useful because of describing the physics of many scientific phenomena and problems, and in their full and/or simplified forms help with the design of aircraft and cars [1], the study of blood flow [2], the analysis of pollution [3], and many other things. Solidification is not an exception [4] , [5] in this context. A great many different models have been proposed over the years that offered reasonable results [6], [7], but each of them assumed some simplifications. None of the results included all of the problems occurring during modeling of this complicated phenomenon. Many of the computation models are subject to some restrictions. For instance, one such restriction is the omission of convection force in liquid metal. Unfortunately, their omission in a numerical model may cause crucial differences between the temperature range achieved in computer simulations, and the temperature of the real casting itself. What is more, due to such a simplification it is not possible to model certain phenomena which are essential factors influencing the quality of castings for example, dopant distribution in the casting or shrinkage during solidification [8].

Simulation tools become indispensable for engineers who are interested in tackling increasingly more complex problems or the ones who are interested in searching larger phase space of process and system variables to find the optimal design. Advances in hardware allow not only to solve the larger tasks (using more detailed grids) but also to describe the problem more accurately. Increasing capacity of computer memory makes it possible to consider growing problem sizes. At the same time, increased precision of simulations triggers even greater load. The increasing complexity of models (by including a more significant number of processes in them) causes problems with the implementation of the models. A solution to the transfer equations causes numerical problems regardless of the chosen discretization method. What is more, numerical methods of solving the Navier-Stokes equations are characterized by the significant time of calculations. That is why modern models must be implemented with the use of technology such as parallel computers [9], accelerated architectures or by using a specific organization of calculations [10], [11].

The Navier-Stokes equations depend on the simulated phenomenon. There may be a need to include a wide range of fluid motion speeds. Whether the focus is on the very convection or the flow of metal in the gating system, due to the high density of the metal, it is not possible to overlook fluid inertia effects. In our work, we propose the use of the stabilized finite element method (FEM) form to solve the Navier-Stokes equations without considering the classic Ladyzhenkaya-Babuska-Brezzi (LBB) consistency condition which can impede obtaining a solution of these equation [12].

In the paper, the results of the computer simulations of solidification with consideration of the liquid phase movement and dimensions of cast and mold are presented. The

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paper includes, too, a brief description of the chosen stages of the numerical model development (e.g., problems with occurring of momentum and continuity equations, as well as conditions in which convection is the crucial factor). All of that is supplemented with figures of the temperature, solid phase, and velocity distribution in different moments of a process lasting.

II. Mathematical derivations

The governing equation for modeling solidification process is based on heat transfer equation with source term:

$$\rho c\dot{\mathbf{T}} + \rho c(\mathbf{u}\cdot\nabla)\mathbf{T} = \lambda\nabla^2\mathbf{T} + \dot{q} \tag{1}$$

where $\mathbf{T}$ is temperature, $\mathbf{u}$ is velocity from convection force, λ is thermal conductivity, ρ is density, c is specific heat, q is heat source along with the heat of solidification and dot over the letter is a time derivative. In the model solving equation (1) the Newton boundary condition on the outer sides of the mold was implemented (heat exchange between the mold and the environment) also, the contact condition for the heat exchange between the mold and the casting. Apparent heat capacity formulation can be written as the following equation:

$$c^*\dot{\mathbf{T}} + \rho c(\mathbf{u}\cdot\nabla)\mathbf{T} = \lambda\nabla^2\mathbf{T} \tag{2}$$

where c^* is the approximation of the effective heat capacity. From different methods of this approximation, the Comini method was chosen:

$$c^* = \frac{1}{n}\left(\frac{\frac{\partial H}{\partial x}}{\frac{\partial T}{\partial x}} + \frac{\frac{\partial H}{\partial y}}{\frac{\partial T}{\partial y}}\right) = \frac{1}{n}\frac{H_{,i}}{T_{,i}} \tag{3}$$

where n is number of dimensions. Due to the assumption that liquid metal is a Newtonian fluid in this model it possible to write Navier-Stokes set of equations as:

$$\rho\dot{\mathbf{u}} + \rho((\mathbf{u}\cdot\nabla)\mathbf{u}) - \nabla p + \rho\mu((\nabla\mathbf{u}) + (\nabla\mathbf{u})^T) + \\ + \rho\mu\frac{f_l}{K_\epsilon}\mathbf{u} = \rho\mathbf{f} \tag{4}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{5}$$

where p is pressure, μ is viscosity, f_l is a liquid fraction, K_ϵ is the permeability of the mushy zone approximated by The Kozeny-Carman equation and $\mathbf{f}$ is a vector of body forces, that arose from buoyancy forces.

The proper set of initial and boundary conditions complements the above equations. Firstly, $\mathbf{u}$ is set as an initial condition, and secondly, the no-slip condition is used between the mold and the cast.

After spatial discretization using the finite element method [13], it can be written as:

$$\begin{aligned} \mathbf{M}'\dot{\mathbf{T}} + (\mathbf{N}'(\mathbf{u}) + \mathbf{K}')\,\mathbf{T} = 0 \\ \mathbf{M}\dot{\mathbf{u}} + (\mathbf{N}(\mathbf{u}) + \mathbf{K})\,\mathbf{u} - \mathbf{G}\mathbf{p} + \mathbf{D}\mathbf{u} = \mathbf{F} \\ \mathbf{G}^T\mathbf{u} = 0 \end{aligned} \tag{6}$$

where $\mathbf{M}$ is a mass matrix, $\mathbf{K}$ is stiffness matrix, $\mathbf{N}$ is a matrix of shape function connected with velocity $\mathbf{u}$, $\mathbf{G}$ is matrix connected with basic functions of the finite elements [14] and $\mathbf{F}$ is vector of body forces.

Equations in that form can be solved with precisely selected finite elements [15]. The strategy which is described in this paper is based on the use of the stabilized Finite Element Method [16]. It makes it possible to avoid limits imposed by the Ladyzhenskaya-Babuska-Breezi condition. SUPG (Streamline Upwind Petrov-Galerkin) and PSPG (Pressure Stabilized Petrov-Galerkin) techniques supply stabilization. Despite the fact that SUPG should reduce solution oscillations occurring due to high velocities, it is still possible to obtain these oscillations because of high gradients of temperature. Thus additionally, it is popular to use a diagonal mass matrix to avoid oscillations caused by high gradients during solidification simulations.

Consideration of the drag force part in stabilization requires special efforts [17]. An approach used in this paper determines stabilization coefficient values by the velocity of the liquid and limits it proportionally to the volume of liquid fraction. During the calculations, the authors assumed a small time step which allowed to use temperature from the previous time step when the temperature was needed to determine actual material properties values. That approach permits to treat solidification equation as linear, which makes for better overall performance. What is more, such an approach allows using a lumped mass matrix in solidification equation [14]. Bearing described assumptions in mind and using Θ scheme for time integration, the final form of equations solved in the applied model is:

$$[\mathbf{M}' + \mathbf{M}'_{SUPG} + \Delta t\Theta(\mathbf{N}'_{SUPG} + \mathbf{K}')]\mathbf{T}^{t+1} = \\ [\mathbf{M}' + \mathbf{M}'_{SUPG} + \Delta t(1-\Theta)(\mathbf{N}'_{SUPG} + \mathbf{K}')]\mathbf{T}^{t} \tag{7}$$

$$[\mathbf{M} + \mathbf{M}_{SUPG} + \Delta t\Theta(\mathbf{N}_{SUPG} + \mathbf{K} + \mathbf{D} + \mathbf{D}_{SUPG})]\mathbf{u}^{t+1} \\ - \Delta t\mathbf{G}\mathbf{p}^{t+1} + [\mathbf{M} + \mathbf{M}_{SUPG} + \Delta t(1-\Theta)(\mathbf{N}_{SUPG} \\ + \mathbf{K} + \mathbf{D} + \mathbf{D}_{SUPG})]\mathbf{u}^{t} = \Delta t[\Theta(\mathbf{F} + \mathbf{F}_{SUPG}) \\ + (1-\Theta)(\mathbf{F} + \mathbf{F}_{SUPG})] \tag{8}$$

$$[\mathbf{M}_{PSPG} + \Delta t\Theta(\mathbf{G}^T + \mathbf{N}_{PSPG} + \mathbf{D}_{PSPG})]\mathbf{u}^{t+1} - \\ \Delta t\mathbf{G}_{PSPG}\mathbf{p}^{t+1} + [\mathbf{M}_{PSPG} + \Delta t(1-\Theta)(\mathbf{G}^T + \mathbf{N}_{PSPG} \\ + \mathbf{D}_{PSPG})]\mathbf{u}^{t} = \Delta t[\Theta\mathbf{F}_{PSPG} \\ + (1-\Theta)\mathbf{F}_{PSPG}] \tag{9}$$

where matrices with $SUPG$ and $PSPG$ are terms supplied by stabilization, Δt is time step and Θ is parameter determining type of time integration scheme.

III. Results

The model described in section II was implemented by authors hereof in C++ language with the use of TalyFEM finite element routines library [18] and PETSc, as a provider of linear algebra algorithms and data structures [19]. The results of calculations taking into account convection are shown for the domain presented in Fig. 1. The boundary conditions utilized the following parameters: Newton boundary condition with the environment temperature equal to 300 K, the heat exchange coefficient was equal to 10 $W/(mK)$ on the bottom wall of the mold, 20 $W/(mK)$ on the left and right wall and equal to 40 $W/(mK)$ on the upside wall of the mold. Continuity condition assumed a value of

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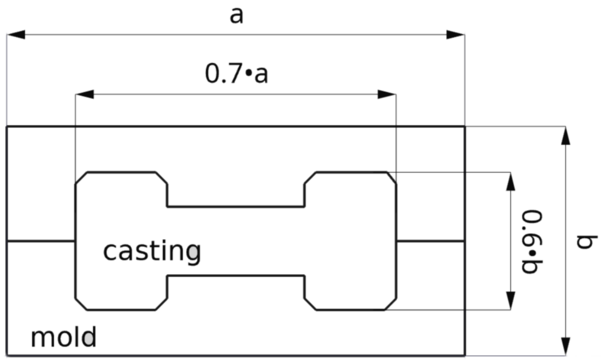

Fig. 1: View of the cast and mold with parameterized dimensions.

1000 $W/(mK)$ for heat transfer through a separation layer between the mold and cast.

A summary of the material properties can be found below in Table I (for casting) and Table II (for mold). That properties correspond on a binary alloy Al-2%Cu.

TABLE I: Material properties for casting

Quantity name	**Unit**	**Value**
Density ρ_s	kg/m^3	2824
Density ρ_l	kg/m^3	2498
Specific heat c_s	$J/(kg\,K)$	1077
Specific heat c_l	$J/(kg\,K)$	1275
Thermal conductivity λ_s	$W/(m\,K)$	262
Thermal conductivity λ_l	$W/(m\,K)$	104
Solidus temperature T_s	K	853
Liquidus temperature T_l	K	926
Solidification temperature of pure component T_M	K	933
Eutectic temperature T_E	K	821
Heat of solidification L	J/kg	390000
Solute partition coefficient k	–	0.125
Viscosity μ	$kg/(m\,s)$	0.004
Expansion coefficient β	$1/K$	0.0001
Secondary dendrite arm spacing K_0	m	$1.4 \cdot 10^{-11}$

TABLE II: Material properties for mold

Quantity name	**Unit**	**Value**
Density ρ	kg/m^3	7500
Specific heat c	$J/(kg\,K)$	620
Thermal conductivity λ	$W/(m\,K)$	40

The computational domain comprised of 64180 nodes and 125972 triangle finite elements. Time step used in time integration was equal to $0.025\,s$, and time integration used a value of Θ equal to 1 (Euler Backward). Total run time for our simulation was $120\,s$. The results of the computer simulation are presented only for the first $15\,s$, $30\,s$ $60\,s$ after which most samples showed no significant convection.

The results for the four instances are presented. All simulations use linear triangular finite elements. Dimensions of each domain are parametrized according to Figure 1. The base case has size of $a = 1.0\,m$ and $b = 0.5\,m$ and is treated as 100%. Other samples have 75%, 50%, and 25% base lengths. Those four cases allow assessing the importance of convection in solidification.

The first series of results present temperature maps for four size of the cast and mold after $15\,s$ (Fig. 2), after $30\,s$ (Fig. 3), and after $60\,s$ (Fig. 4) the time duration of simulations. The more casting size, the more visible is the effect of convection observed as a fluctuation of temperatures during the solidification process. The effect of convection is well visible at the beginning of simulations. With increasing time, the effects of convection are less evident. In each case, according to prediction, the symmetry of results is easily observable.

Corresponding solid fraction and velocity maps are presented in Fig. 5, 6, 7, and in Fig. 8, 9, 10, respectively. The liquid phase movement influence on course of solidification process. The bigger size of the cast the more effect of the convection, consequently the slower heat emmision and the slower solidifying.

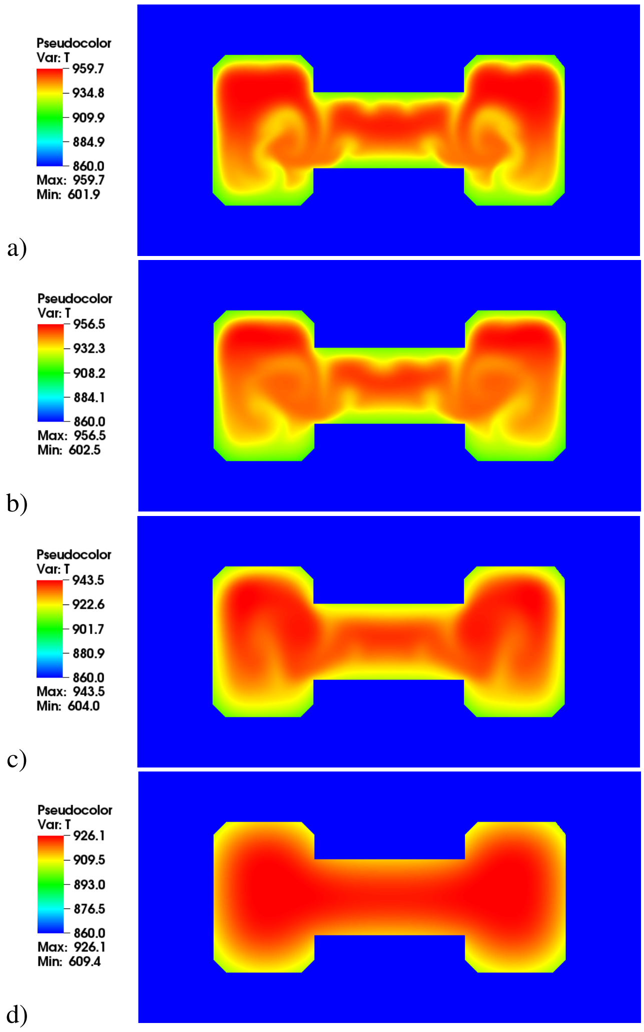

Fig. 2: Temperature distribution after 15 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

IV. Summary

The paper discusses the problem of convection in solidification simulations. It presents the influence of liquid phase movement on the solidification process. Included computations show, that influence of convection during the solidification process depends on the casting size and affect results concerning the temperature and solid fraction maps. The tools development for numerical computing are to

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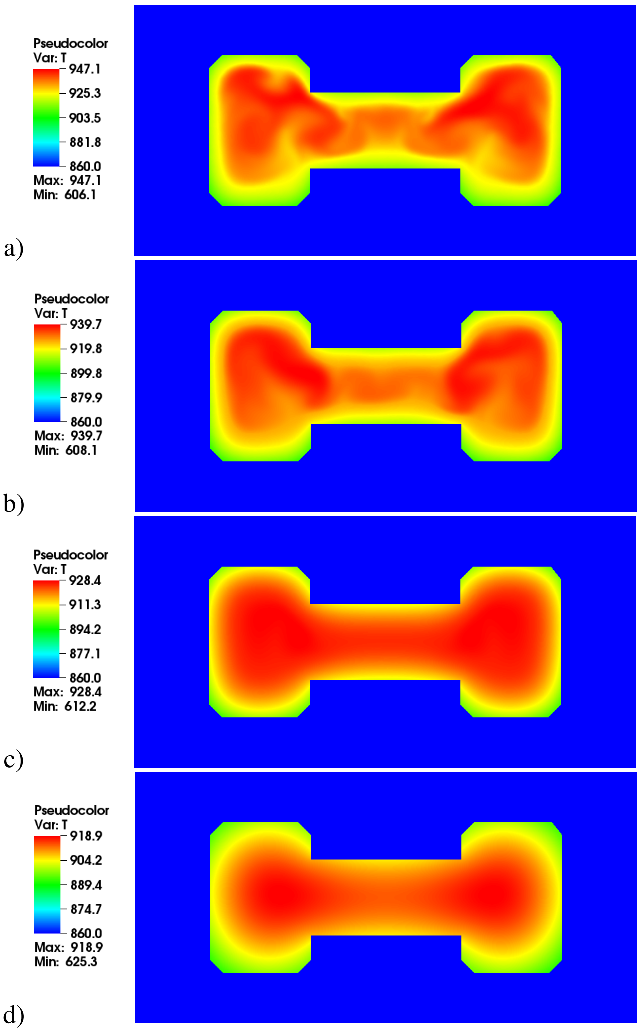

Fig. 3: Temperature distribution after 30 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

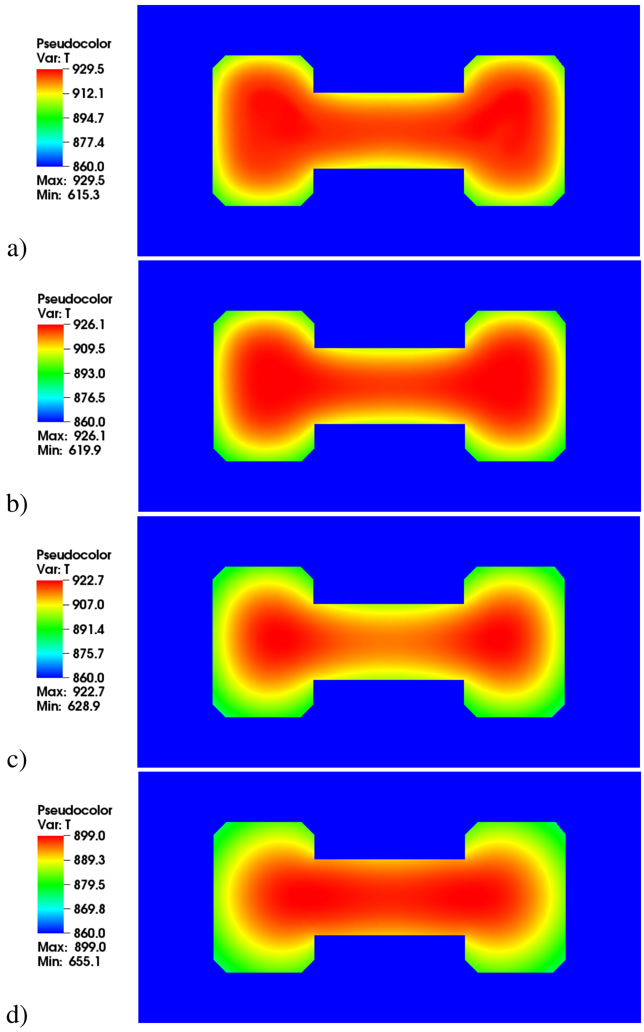

Fig. 4: Temperature distribution after 60 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

make them i) fast, ii) cheap (simulations on workstations), iii) flexible (general-purpose solver), iv) accurate (adaptive error control) [20]. The authors software, which is still in development, satisfies all of these conditions. Future work plans include an experimental comparison of results as the presented model has so far been checked only against benchmark problems.

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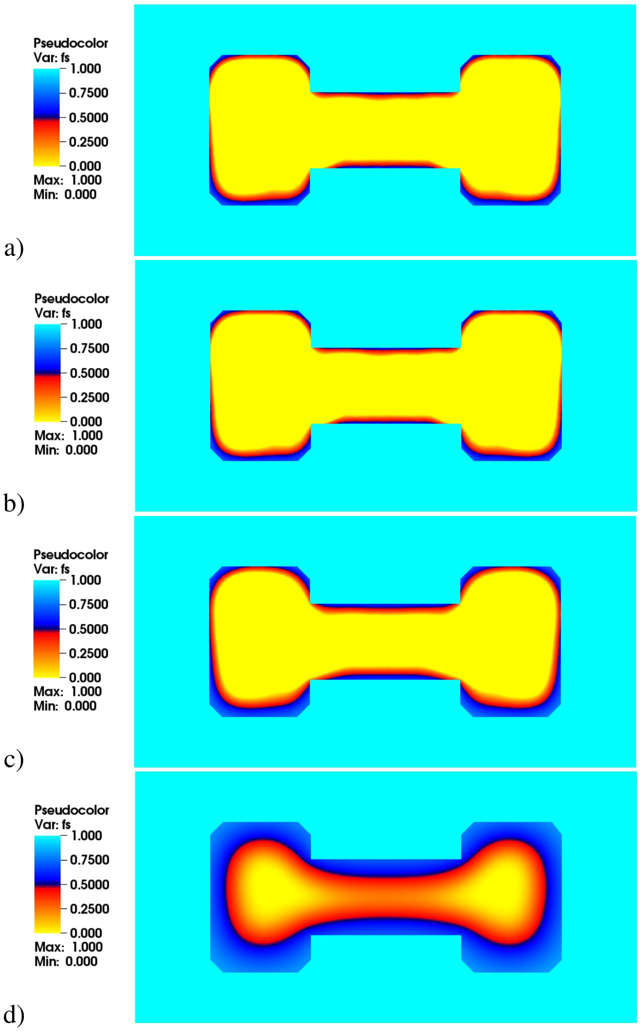

Fig. 5: Solid fraction distribution after 15 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

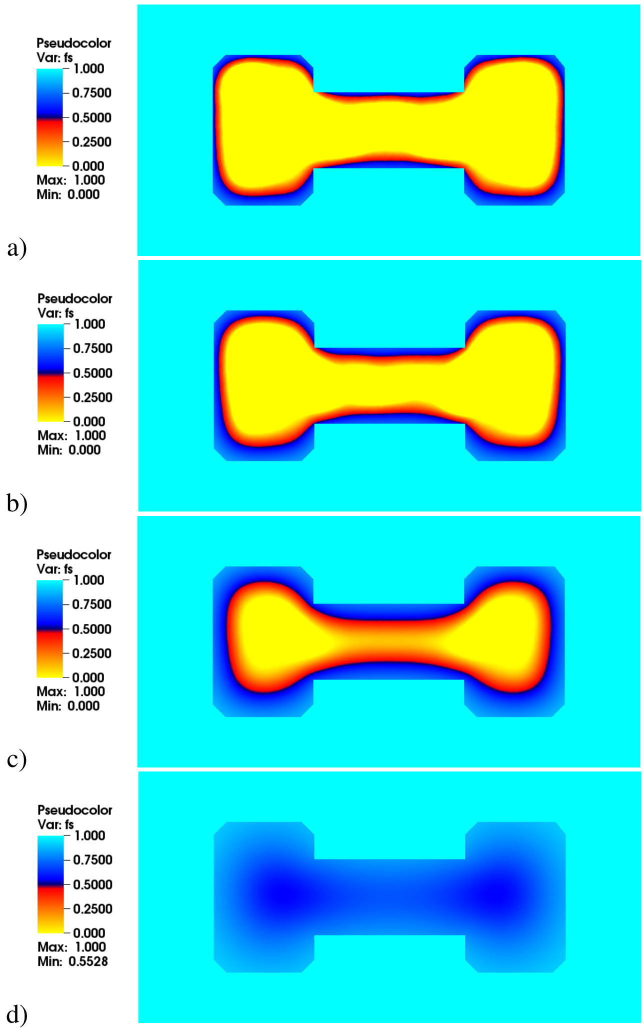

Fig. 6: Solid fraction distribution after 30 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

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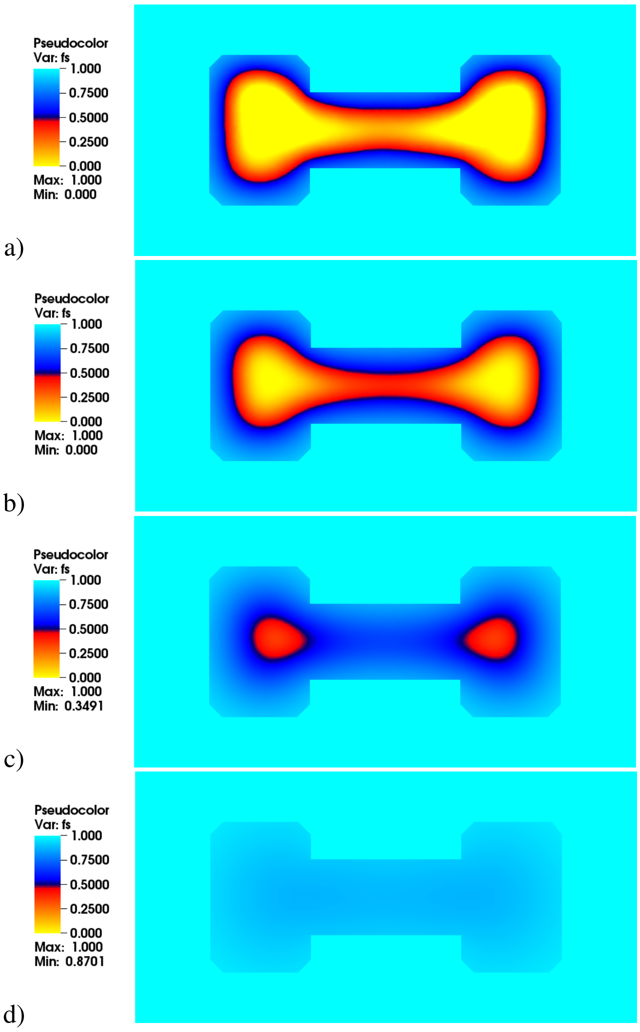

Fig. 7: Solid fraction distribution after 60 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

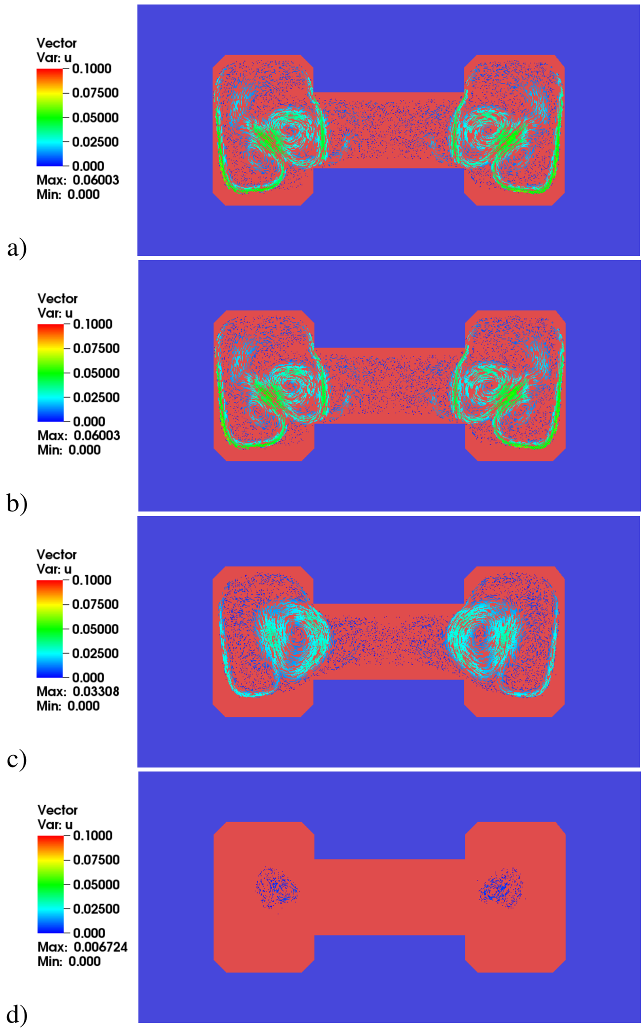

Fig. 8: Velocity vectors distribution after 15 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

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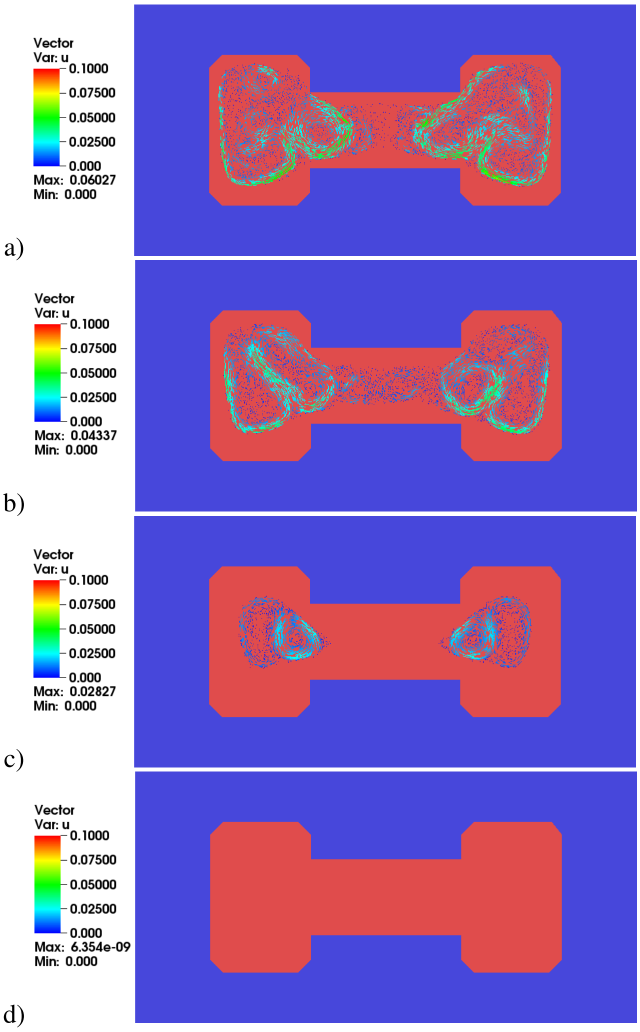

Fig. 9: Velocity vectors distribution after 30 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

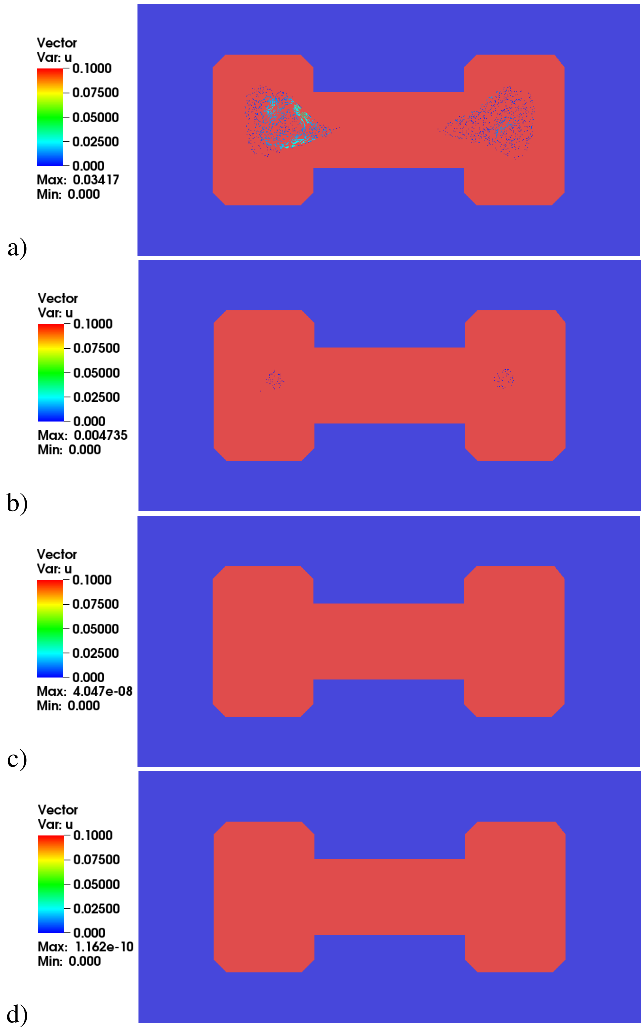

Fig. 10: Velocity vectors distribution after 60 seconds for a) 100%, b) 75%, c) 50%, and d) 25% dimensions of considered domain.

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