Implementation of regularized equations for the disk pump simulation problem in OpenFOAM

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***Abstract*—The creation of an effective pump that is able to maintain blood circulation in the heart with appropriate medical indications is undoubtedly an crucial task. The first versions of such devices are currently being created and tested on the basis of IFPM SB RAS, Novosibirsk. The work is devoted to the pump numerical simulations in order to optimize its parameters. The equations of viscous incompressible fluid flow are used for this purpose. Numerical algorithm is based on the regularization of the initial equations, which applies a finite volume method that avoids limiting procedures and includes controlled numerical dissipation. Calculations are carried out within the open software package OpenFOAM installed in ISP RAS. Unsteady flow in the pump is studied.**

***Index Terms*—hydrodynamics, regularized equations, numerical simulation, disc pump, OpenFOAM, incompressible flows, thrombosis.**

I. Introduction

The disk pump prototype consists of a body 1 and a rotor 2 placed in it (fig. 1). As the rotor rotates, the liquid is sucked through the inlet 3 and after receiving an acceleration in the rotor, it is ejected through the outlet 4.

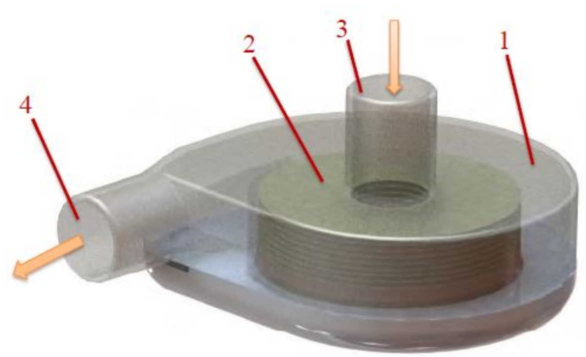

Fig. 1. Disk pump model for blood pumping.

By now simulation attempts this device with the use of analytical approaches and limited simulation attempts using commercial packages do not allow to optimize the device, as shown in [1].

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The use of the open software package OpenFOAM and included in it the original computational core based on the regularized equations of hydrodynamics will allow to:

- investigate the mechanics of the variable fluid flow in the pump to support the blood motion in the approximation of direct numerical simulation;
- investigate the possibility of thrombosis in the flow in pump.

The paper presents several stages of the building the model describing a disk pump consisting of two disks and nine disks, and its implementation in the framework of the OpenFOAM complex. The models include the spatial calculation area setting, the configurations of which correspond to a simplified form of the real geometry of the disk pump and constructing the equation system in the laboratory coordinate system in collaboration with the boundary conditions. Computational data for simplified two-disk model and a full pump model with nine disks are presented taking into account nonstationary flow and distributions of viscous shear.

II. Simulation of a disk pump consisting of two discs

A. Mathematical model and geometry of the problem

The problem is solved using regularized hydrodynamic equations, or so-called quasi hydrodynamic (QHD) equations, which were derived by Y.V. Sheretov in 1996 and can be found, for example, in [2], [3] and [4]. The regularized continuity equations and momentum balance for isothermic incompressible flow have the following form:

$$\begin{cases} div\,(\vec{u}-\vec{\mathrm{w}}) = 0, & (1)\\ \dfrac{\partial \vec{u}}{\partial t} + (\vec{u}-\vec{\mathrm{w}})\cdot \vec{\bigtriangledown}\vec{u} + \dfrac{1}{\rho}\vec{\bigtriangledown}p = \dfrac{1}{\rho}div\Pi, & (2)\end{cases}$$

Here $\rho = const > 0$ is an average value of the density, $\vec{u} = \vec{u}\,(\vec{x},t)$ is a hydrodynamic velocity, $p = p\,(\vec{x},t)$ is a hydrodynamic pressure. The viscous tensor Π and additional velocity $\vec{\mathrm{w}}$ are calculated as:

$$\vec{\mathrm{w}} = \frac{\tau}{\rho}\left[\rho\left(\vec{u}\cdot\vec{\nabla}\right)\vec{u} + \vec{\nabla}p\right], \qquad (3)$$

$$\Pi = \Pi_{NS} + \rho\vec{u}\otimes\vec{\mathrm{w}}, \qquad (4)$$

$$\Pi_{NS} = \eta\left[\left(\vec{\nabla}\otimes\vec{u}\right) + \left(\vec{\nabla}\otimes\vec{u}\right)^T\right], \qquad (5)$$

where η is a coefficient of dynamic viscosity.

Regularized equation system (1) – (5) differs from Navier-Stoks equations by terms with small parameter τ as a coefficient. Terms in τ act as a regularizers and allow to use a simple numerical method without limitors to solve the system (1) – (5). The stability and accuracy of numerical results depend of the value τ. According to computational practice, it is convenient to choose τ an order of magnitude inversely proportional to the Reynolds number Re:

$$\tau \sim \frac{\tau_0}{Re}. \qquad (6)$$

The computational domain and spatial grid was created in the open integrable Salome platform. The geometry of the computational domain is shown in fig. 2 and fig. 3 (1 and 2 are the outlet and inlet respectively, 3 and 4 are the upper and lower disk respectively).

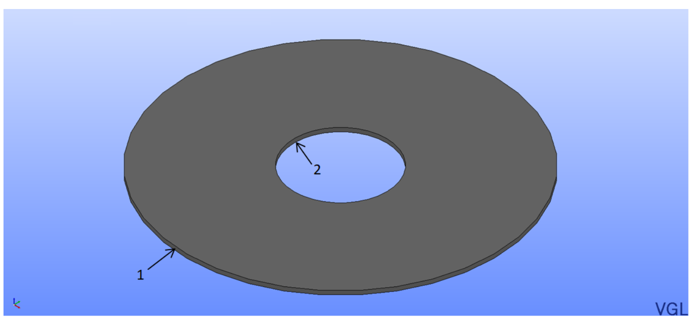


Fig. 2. Two disk pump model, volume view.

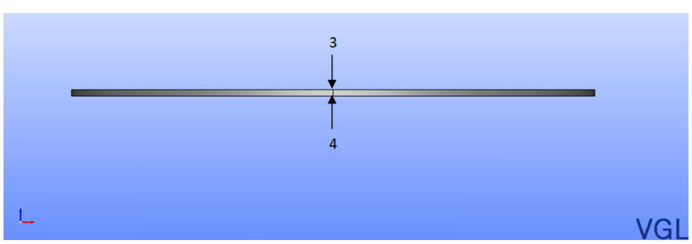
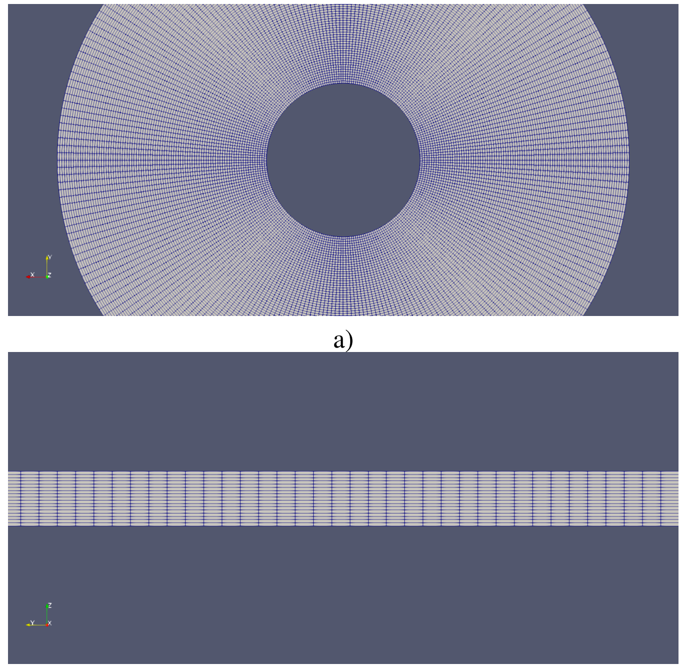


Fig. 3. Two disk pump model, side view.

The spatial grid in the computational domain was constructed using the Salome (fig. 4). The number of cells is approximately equal to $3.4\cdot10^5$ with number of cells in r, z and angular directions equals to $200\times17\times100$.

B. Parameters of the calculations

The parameters used in the calculations correspond to the data given in [1].



a)

b)

Fig. 4. Grid for calculation, view along the z axis – (a) and side view – (b).

Designed parameters of the problem: the distance between disks is $2h$. The inner and outside radii of the disks are a and b respectively. In this problem $a = 6mm$, $b = 20mm$, and the gap between disks is $2h = 0.5mm$.

Parameters of the model mixture (40% glycerin + 60% water): dynamic viscosity coefficient $\eta = 3.7\cdot10^{-3}\frac{kg}{m\cdot s}$; density $\rho = 1100\frac{kg}{m^3}$.

The parameters of the pump (2 discs): discs rotation speed $\Omega = 1500\frac{r}{min}$; the flow intensity between the discs $Q_1 = 0.27\frac{l}{min}$.

The average velocity in the cross-section with a radius r is calculated by: $u(r) = \frac{Q_1}{S(r)} = \frac{Q_1}{2\pi r2h}$; Reynolds number: $Re = \frac{\rho ul}{\eta}$, $Re_\Omega = \frac{\Omega l^2\rho}{\eta}$; a characteristic time $\tau_0 = \frac{l}{u(a)}$, $\tau_{0\Omega} = \frac{l}{\Omega a}$, where l is a characteristic size of the computational domain ($l = 20mm$). These values are presented in the table I.

It is necessary to choose the regularization parameter for calculations. In non-dimensional form as shown in section II-A: $\tau \sim Re_\Omega^{-1}$. We obtain the values for τ taking the values of the Reynolds numbers Re and Re_Ω from section II-B, which are shown in the table II.

TABLE I
VALUES OF QUANTITIES SPECIFIC TO THE MODEL

Quantities	$Q_1 = 0.27\frac{l}{min}$, $\Omega = 1500\frac{r}{min}$
$u_r(a)$, $\left[\frac{m}{s}\right]$	fig. 5
Re	1500
Re_Ω	20000
τ_0, $[s]$	0.08
$\tau_{0\Omega}$, $[s]$	0.02

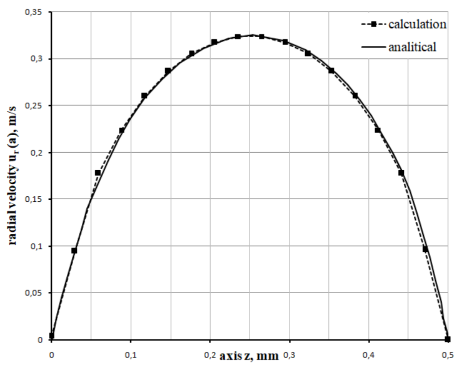


Fig. 5. Comparison of input profiles of the radial velocity, the rotational velocity of the disk $\Omega = 1500\frac{r}{min}$.

TABLE II
THE VALUES OF THE PARAMETERS OF REGULARIZATION

	$Re = 1500$	$Re_\Omega = 20000$
τ, $[s]$	$5 \cdot 10^{-5}$	$1 \cdot 10^{-6}$

C. Results of calculations

The flow in the gap between rotating flat disks is considered. The obtained results are compared with the analytical solution given in [1]. Fig. 6 shows radial velocity profiles at the outlet of the gap between the flat discs $(r = b)$ for the rotational speed of the discs equals to $1500\frac{r}{min}$.

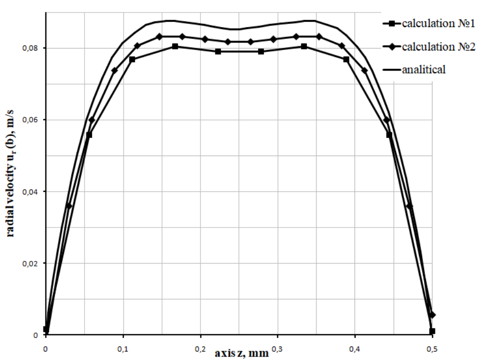


Fig. 6. Comparison of output profiles of the radial velocity, the rotational velocity of the disk $\Omega = 1500\frac{r}{min}$. Grid for calculation №1 consists of $2.88 \cdot 10^5$ cells, and for calculation №2 consists of $3.4 \cdot 10^5$ cells.

It is necessary to reduce the time spent by blood inside the pump to optimize the parameters of the pump. For this purpose in [1] calculations of trajectories of erythrocytes of blood in a gap between disks were carried out. Numerical calculations also show that at the rotation speed of the disks $\Omega = 1500\frac{r}{min}$ the integer number of revolutions of the particle is 2. The trajectories of both calculations are shown in fig. 7.

The numerical calculation coincides with the analytical solution as seen in fig. 6 and fig. 7. The mesh independence to the analytical solution is shown in fig. 6. Consequently, there is a qualitative and quantitative correspondence between the analytical solution and the numerical calculation, which

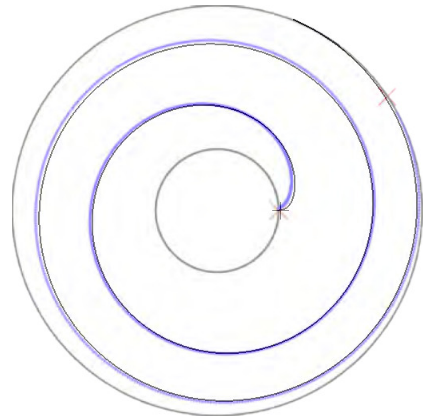


Fig. 7. Trajectories of motion of liquid particles from analytical results (blue), shown in [1], and from the present numerical experiment (black).

describes the motion of the fluid in the gap between the two disks.

D. Head-capacity curve

It is necessary to perform additional calculations on various input data presented in table III to construct the head-capacity characteristics.

TABLE III
VALUES OF Ω AND Q_1 FOR ADDITIONAL CALCULATIONS

$\Omega = 1500\frac{r}{min}$	$\Omega = 2000\frac{r}{min}$
$Q_1 = 0.25\frac{l}{min}$ $Q_1 = 0.1\frac{l}{min}$	$Q_1 = 0.45\frac{l}{min}$ $Q_1 = 0.25\frac{l}{min}$ $Q_1 = 0.1\frac{l}{min}$

Some numerical instabilities were seen at the exit of the gap between disks because of relatively low shear viscosity coefficient. The computational domain was increased by extending the input and output area as a first step to overcame this problem (fig. 8). The grid looks similar to the fig. 4. The number of cells in r, z and angular directions equals to $240 \times 17 \times 84$.

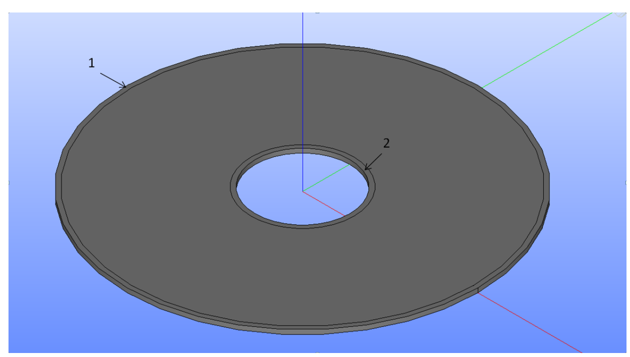


Fig. 8. View of the improved calculation area. 1 is an additional output area, 2 is an additional input area.

As a second step to overcome the numerical instabilities we implemented the calculations with initial conditions, corresponding to successively increased Reynolds numbers to the desired value. Four additional calculations were carried out with $Re = 200, 2000, 4000, 9000$. The variant with $Re = 200$ was used as an initial condition for variant with $Re = 2000$, and so on up to the desired variant with $Re = 20 \cdot 10^3$.

Values for the flow-discharge characteristic were obtained (fig. 9) as a result of the calculations. The dependence was linear, the data from the numerical calculation qualitatively and quantitatively coincide with the values from the analytical calculations described in [1].

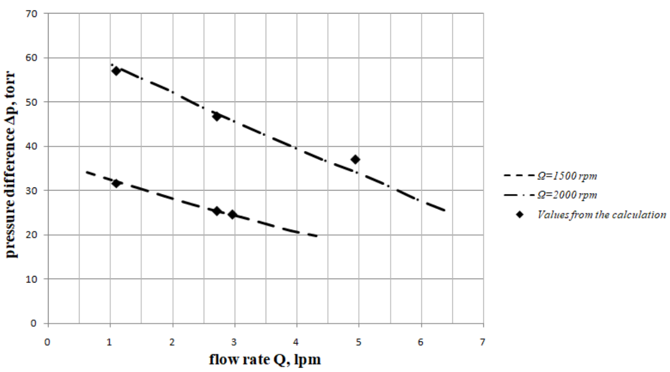
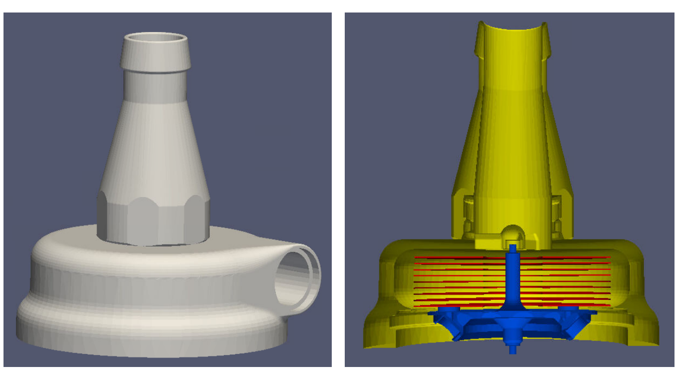


Fig. 9. Comparison of the head-capacity curves taken from [1] for $\Omega = 1500$ rpm and 2000 rpm with the values of present calculations

III. Simulation of a disc pump consisting of nine discs

A. Geometry and grid of the computational domain

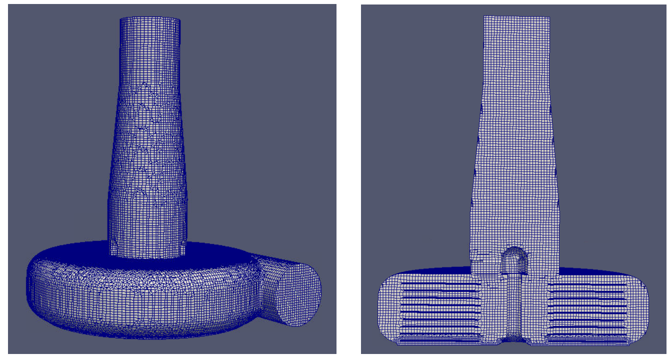
The model is a pump body, input and output channels, rotor, which consists of 9 smooth disks (fig. 10). The outside radius of the disks is 20 mm, inner is 6 mm, thickness is 0.1 mm, the distance between the disks is 0.5 mm. The diameters of the input and output holes are the same and equal to 12 mm.



a) b)

Fig. 10. a) is a volume view, b) is a sectional view.

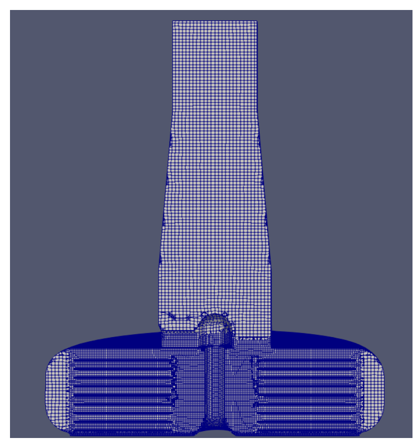
The first computational spatial grid contained approximately $4.2 \cdot 10^5$ cells for all the pump and particularly disks area includes 2 cells between disks surfaces, 145 in height, 50 along a radius (fig. 11). This grid was built using the automatic grid builder snappyHexMesh based on OpenFOAM.



a) b)

Fig. 11. a) is a side view of calculation area, b) is a sectional view of calculation area.

Due to the appearance of the nonphysical oscillations an improved spatial grid with additional condensation in the disk region was constructed (fig. 12). The number of cells is approximately equals to $1.3 \cdot 10^6$ for all the pump and particularly disks area includes 5 cells between disks surfaces, 180 in height, 90 along radius. This spatial grid was also built using the snappyHexMesh grid builder.



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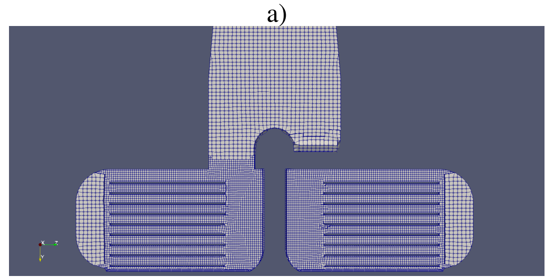


b)

Fig. 12. a) is a sectional view of calculation area, b) is an increased area.

A small number of cells (approximately 0.5%) that had a non-hexahedral form appeared in the created computational mesh. In the considered version of the program, the features of the numerical algorithm implementation assume the use of cells of the correct hexahedral form, providing the required approximation of the τ – terms. Therefore, it was decided to split the entire grid into two sets. In the first set the values of the fields in the cells with a hexahedral structure are calculated using the central difference scheme, and in a second set of the mesh with non-hexahedral structure the upwind scheme is used.

B. Variants of calculations

Calculations are made with parameters which taken from section II-B, and the values are taken from tables IV, V. The calculations are performed at first for a small Re number, specifically $Re = 2000$ and than calculated flow pattern was used as an initial condition for the next variant with $Re = 4000$, as for the variant with two disks, and so on up to the desired variant with $Re = 2 \cdot 10^5$.

TABLE IV
VALUES OF QUANTITIES SPECIFIC TO THE MODEL

Quantities	$Q = 4.07\frac{l}{min}$, $\Omega = 1500\frac{r}{min}$
u_{in}, $\left[\frac{m}{s}\right]$	0.6
p_{out}, $[Pa]$	10^4
Re	5000
Re_Ω	200000
τ_0, $[s]$	0.3
τ_{0_Ω}, $[s]$	0.04

TABLE V
VALUES OF REGULARIZATION PARAMETER

	$Re = 5000$	$Re_\Omega = 200000$
τ, $[s]$	$6 \cdot 10^{-5}$	$2 \cdot 10^{-7}$

C. Results of calculations

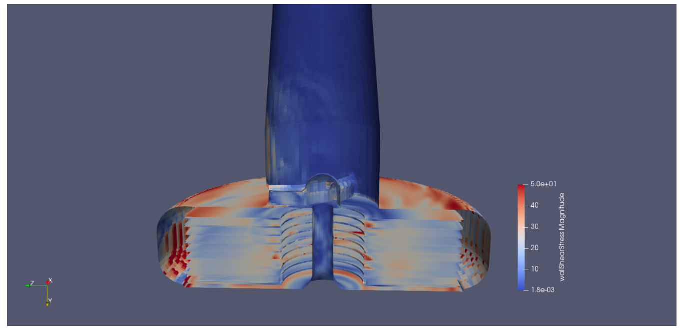
The values of the shear stress modulus on the internal surfaces of the pump were obtained as a result of calculations for $\Omega = 1500\frac{r}{min}$ and $Q = 2.75\frac{l}{min}$. As an example, its values at three different time moments with intervals of $0.14s$ and $0.05s$ are shown in fig. 13. This figure shows complicated non-stationary character of the flow in the disk pump.

The values for the head-capacity curve are shown in (fig. 14). It is necessary to perform additional calculations on different input data presented in table VI to construct the head-capacity curves. The both head-capacity curves turned out to be linear, which confirms the correct operation of the program.

TABLE VI
THE VALUES Ω AND Q FOR ADDITIONAL CALCULATIONS

$\Omega = 1500\frac{r}{min}$	$\Omega = 3000\frac{r}{min}$
$Q = 1.5\frac{l}{min}$ $Q = 2.75\frac{l}{min}$	$Q = 3.73\frac{l}{min}$ $Q = 5.0\frac{l}{min}$ $Q = 6.5\frac{l}{min}$

The trajectory of the particles in the disk pump is shown in fig. 15. This example shows how the particles move in the pump, without falling into the zone of stagnation and separation of the flow.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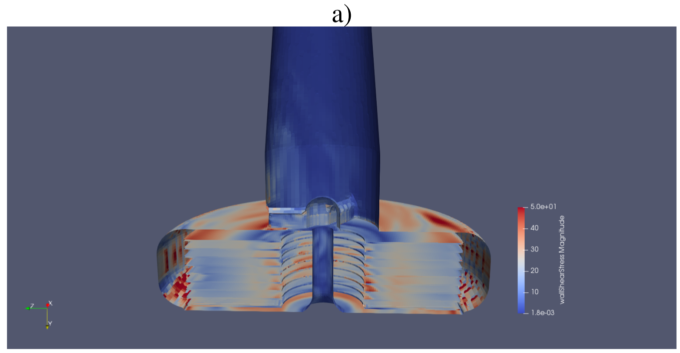
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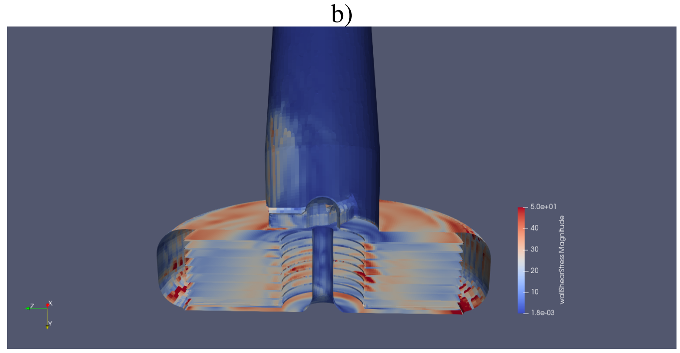

c)

Fig. 13. Field of the module of shear stress at different time moments: $t_a < t_b < t_c$.

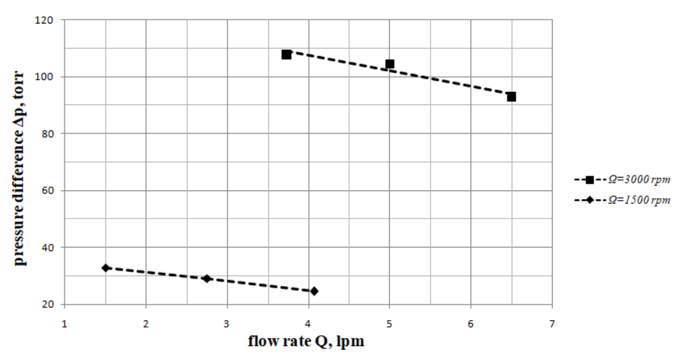


Fig. 14. Comparison of the head-capacity curve taken from [1] for $\Omega = 1500$ rpm and 3000 rpm with the values from the present calculations

As a result of numerical modeling, a complex picture of the fluid flow was obtained, due to the complex geometric shape of the pump and the presence of moving disks. There are particles

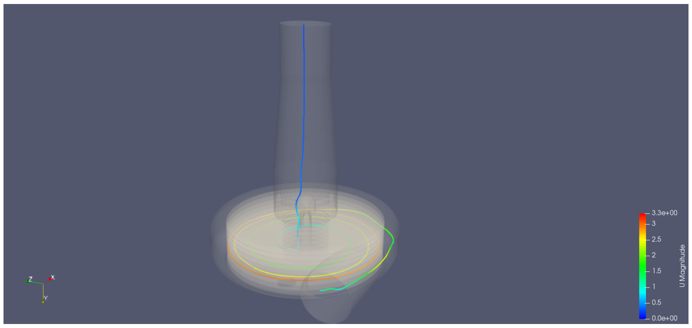


Fig. 15. Example of a particle trajectory of the particles: $\Omega = 1500\ rpm$ and $Q = 3.63\frac{l}{min}$.

that deviate from the above motion. Their trajectories are shown in fig. 16. Figures show additional vortices in different areas of the pump, which can later lead to thrombosis.

IV. Summary

The model of viscous incompressible fluid flow in the flow part of the disk pump of blood circulation maintenance is developed. The model is verified comparing computational results with analytical solution for a simplified problem of a flow in a thin gap between two rotating disks. Numerical convergence is obtained.

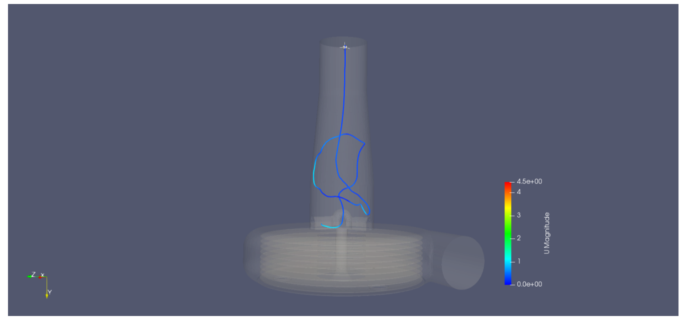
The described mathematical model is based on regularized equations of hydrodynamics, named quasi hydrodynamic (QHD) system. These equations are a generalization of the Navier-Stokes equations and contain additional dissipative terms that depend on the regularization parameter τ. So QHD equations can be regarded as smoothed hydrodynamic equations.Numerical algorithms based on these equations include a controlled, physically justified numerical dissipation determined by a single variable parameter τ in contrast to the classical schemes for solving the Navier-Stokes equations. This parameter is selected depending on the problem statement and on criteria such as Reynolds number Re.

The paper proposes an efficient method for numerical simulation of the problem of viscous incompressible fluid flow in a disk pump at high Re numbers.

Since the Reynolds numbers in the pump flow are sufficiently high, to start the calculations we implemented the series of successive approximations of initial conditions. The first approximation corresponds to the number Re, which describes the laminar flow and is much smaller than a required value. For the next variant with increased Re number the obtained flow field is used as an initial condition, and so on. With each iteration, the Re value increases until it is equal to a required value.

The computational technique includes the following steps:

- selecting an initial value τ that satisfies the following condition: $\tau \lesssim \frac{\tau_0}{Re}$, where τ_0 is a characteristic time;
- setting the initial conditions corresponding to a small number of Re. The chosen Reynolds number must satisfy the requirement for τ – terms;



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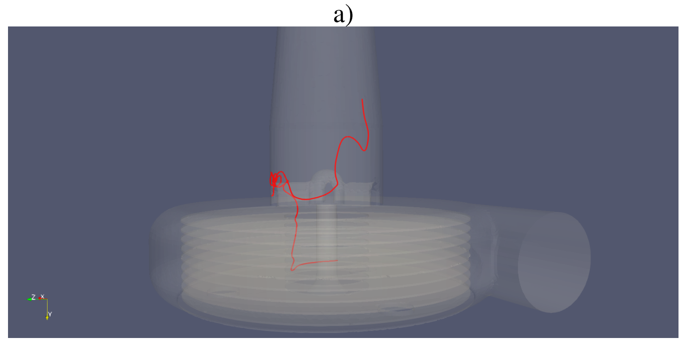

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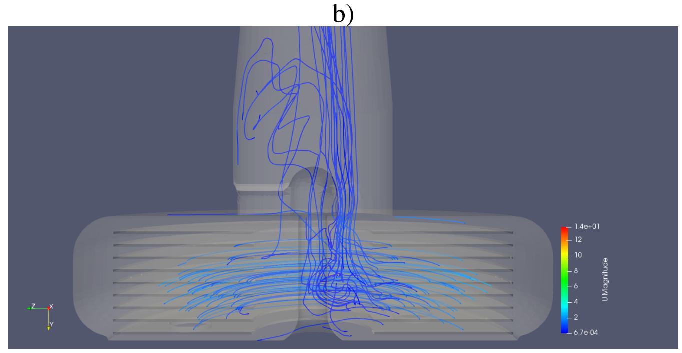

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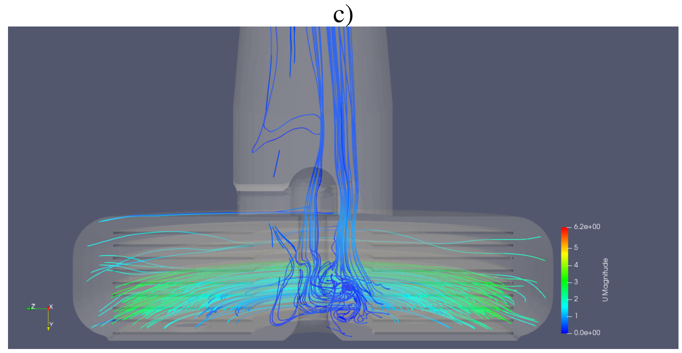

d)

Fig. 16. Examples of particle trajectories in disk pump: $\Omega = 1500\frac{r}{min}\ rpm$ and $Q = 3.63\frac{l}{min}$; (a), (b) are the motion of a single particle, (c), (d) are the motion for 50 particles.

- variation of the Re numbers using the viscosity coefficient.

The stability of the explicite numerical scheme is related with the value of regularization parameter τ. The time-step of computational algorithm approximately can be estimated as $\triangle t \approx 0.25\tau$, where for the problem in hand τ approximately equals to characteristic hydrodynamic time. For extremely high τ the algorithm fails, for extremely small τ a time step became too small. An optimal parameters of the calculations is found by computational experience.

Empirically, it was found that for the effective operation of the QHD algorithm, it is necessary to provide a condensation of the grid of a certain spatial scale, where spatial step decreases with increasing of Reynolds number. If this condition is not satisfied, non-physical oscillations appear in the numerical solution.

In the considered version of the program the numerical algorithm implementation assume using cells of the correct hexahedral form, providing a correct approximation of the finite-difference terms including τ – terms. To approximate the convective terms of QHD equations on cells of irregular shape (non-hexahedral, strongly elongated, skewed, etc.), and to stabilize the solution the upwind scheme was used, instead of central-difference scheme with τ – regularisers.

The proposed method of numerical simulation of the disk pump flow is based on the use of the QHD algorithm implemented in the QHDFoam solver based on the open source library OpenFOAM. Poisson equation for pressure is solved by nonlinear conjugate gradient method included in OpenFOAM library with the accuracy approximately 10^{-7}. Presented version of the algorithm is implemented in parallel regime using from 12 to 36 processors.

During the development of the technique, the QHDFoam algorithm is verified on the problem of incompressible viscous flow in the gap between two rotating disks. A series of calculations are carried out in the gap between two discs at different flow intensities of the pumped liquid and various rotation speeds of the discs. The qualitative and quantitative correspondence of the analytical solution presented in [1] with the results of numerical calculations for the output radial velocity profile are established. Particle trajectories and head-capacity curves were also obtained.

To study the flow in the disk pump to maintain blood circulation, the developed technique was used. The considered part of the pump includes the input channel, the working part consisting of nine disks, and the output collector in the form of a ”snail”.

The spatial grid of the computational domain is constructed using the automatic grid builder of the OpenFOAM package – snappyHexMesh. The number of cells is approximately equal to $1.3 \cdot 10^6$, the dominant cell type has a hexahedron of regular shape.

As the result of numerical simulation of a disk pump the unsteady picture of fluid flow has been obtained. This flow contains zones of flow separation and stagnation that indicates a rather complex nature of the fluid flow in the pump. The head-capacity curve is constructed on the basis of the calculated hydrodynamic fields. A qualitative correspondence between the head-capacity curve of the numerical calculation and the experiment described in [1] is obtained. The discrepancy between the head-capacity curves in the calculation and in the experiment can be explained by the difference between the model of the disk pump and the parameters of the test bench, which are described in [1].

To assess the probability of blood clots, the values of viscous stresses on the inner surfaces of the disk pump were calculated. The values of viscous stresses in the human body should be in the range from 40 to 200 Pa (the values are taken from [1]). In the calculations on the inner surfaces of the disk pump the values do not exceed 50 Pa for disc rotation velocity $\Omega = 1500\ rpm$, and for $\Omega = 3000\ rpm$ the values do not exceed 150 Pa.

Thus, as a result of the computational experiment by means of QHD algorithm, hydrodynamic fields of velocity and pressure in the flow part of the disk pump were obtained, separation zones and stagnation zones were studied, flow – pressure characteristics for different speeds of rotation of the disks were obtained. The prediction of values of viscous stresses on the surfaces of the disk pump was made. The calculated values of viscous stresses are within the permissible range, ensuring the safe operation of the human circulatory system.

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