

## Numerical modelling of the opening process of the three-coating aortic valve

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NUMERICAL MODELLING of the three-coating human aortic valve is the objective of the paper. The proposed approach is used to select the material properties and the thickness of outer coating of the valve, which are required to obtain the proper work of the valve, which in the present paper is considered as the opening process. Following the previously developed model of the monocoating leaflet of the natural human aortic valve, the model of three-coating valve is prepared. Finite element method (FEM) and sensitivity analysis are used to solve the formulated and selected problems. Two methods of estimation of the valve opening process in numerical models are elaborated on the basis of experimental studies.

**Key words:** finite element method, aortic valve, sensitivity analysis, opening process, buckling pressure, three-coating leaflet.

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### 1. Introduction

THE MONOCOATING FEM MODEL of a leaflet of a natural human aortic valve was introduced in [1] on the basis of REUL's [2] physical equations and literature research. Using the results of simulations with the developed model, the sensitivity analysis was applied and the values of geometrical parameters of the leaflet of natural human aortic valve were specified.

Recently, a tendency is observed to create a mechanical valve, whose geometry is based on the natural valve. This prosthesis is often made of a synthetic material, for example of polyurethane (PU).

PU is planned to be used as a constructional material of the blood chamber. It has been found that the blood clot formation proceeds in the polyurethane/blood contact area and the polyurethane is subjected to degradation. Therefore, there is a necessity to modify the surface of polyurethane by covering it with a biocompatible coating. The TiN deposited by PLD (pulsed laser deposition) method is supposed to improve not only the material properties of coated specimen, but also the biocompatibility. The main advantage of using the PLD method is low temperature of the deposition process (room temperature), which does

not change the properties of the substrate (PU). The disadvantage of applying the TiN coatings on polyurethane is reaching high values of compressive stresses (residual stress equals about 10 GPa), because of the character of deposition process. Therefore, the best future model of synthetic aortic valve should consider the distribution of residual stresses, which are experimentally examined after the deposition process. This experimental fact leads to a high risk of degenerative failure of these coatings, especially on polyurethane/TiN contact region. From the theoretical point of view, the loaded thin coatings have the highest probability of irreversible failure on the not directly loaded surface (opposite side). The tensile stress concentration on the opposite side of the loaded surface of the coating is thought to be one of the main reasons responsible for the degeneration.

Thus, the project of a model of leaflet of human aortic valve prepared by the Authors of the present paper is extended, because each of the identical leaflets of valve has a three-coating structure: TiN/PU/TiN. The model also satisfies the basic conditions [2] required for the physical construction of the human aortic valve. The decision parameters of proposed construction are determined by the minimal physiological buckling pressure, dependent on the material properties of each coating (the Young modulus) and on the geometry of leaflet (the thickness). The main problems, which are solved in the present work, are related to:

1. Scaling – the real dimensions of coatings are very small (nano-scale). The known theory of mechanical similarity [3] is easy to use for the 2D FEM solutions, but the 3D FEM models need additional computations to define the correct transitions between parameters in different scales. In the present work, the scaling parameters are: the buckling pressure during the valve opening process as the input parameter and the displacement of the loaded model of leaflet as the output parameter.
2. The new construction, whose mechanical response depends on the geometrical ratio – the quotient between the thickness of the deposited outer coating and the thickness of the whole leaflet. The value of Young's modulus of the outer deposited coating is changed for each defined geometrical ratio.
3. High mesh density, which leads to large scale computations. The real, very small thickness of the outer coatings and, in consequence, the very small geometrical ratio is difficult to reach using the standard FEM code without the large scale solutions. It is due to the millions of elements, which should have to be generated to create the fine mesh through the thickness of each coating. This problem is solved by selecting the meshes with optimal density.

Development of the TiN/PU/TiN mathematical model of the human aortic valve is the main objective of the present work using the ADINA FEM code. Assuming the displacement of the leaflet reached in its characteristic point as

the output of the FEM model, the sensitivity coefficients for this parameter with respect to the Young modulus of the outer coating are calculated. The next objective is to estimate the opening process of the human aortic valve for different values of the Young modulus and thickness of the outer coating. It is caused by the fact that the material properties of TiN depend closely on the type of deposition technique and on the conditions used in deposition process, thus the values of Young's modulus of the model have to be meaningfully diversified in the simulations.

At the stage of present research, the most important from Author's point of view is to determine the best elastic properties of coatings and the thickness of outer coatings of aortic valve leaflet, to obtain the minimal values of buckling pressure and the smallest values of stress in the leaflet. Therefore, the opening process, which is limited by the buckling pressure, is considered as the most important one. Additionally, researchers who prepare the physical tests, which are performed for valves, focus mostly on analyzing the opening process of valve and introduce all the details concerning the opening process into "valve's passport". On the basis of physical observations and investigations, the model of the valve is constructed in the present paper.

Finally, two methods of estimating the opening process of valve are elaborated on the basis of the approach, which is used to calculate the parameters introduced in the "valve's passport" during testing in the heart simulator. The opening process of TiN/PU/TiN model of leaflet of human aortic valve model is defined by the displacement leaflet opening reached in its characteristic point (the direct output parameter) and the area of the leaflet opening calculated by comparison the meshes before and after loading (buckling pressure) in the AutoCad program. This project should be extended in the future and dedicated to more problems of valve mechanical working. From numerical point of view, modeling of the closing process and coaptation properties of the leaflets is not possible in commercial FEM codes. Thus, it is needed to elaborate the FEM code, which enables to link fluid and solid meshes, as well as to perfectly rebuild meshes when the elements are too deformed. After remeshing, the volume of mesh should remain the main and these two meshes still have to be connected. The proposed solution is to define the hybrid meshes (also hp adapted meshes) in the fluid-solid contact area.

## 2. Aortic valve

The heart consists of two pumps: the right side supplying the lungs and the left side, pumping oxygenated blood through the body. The pumps consist of a collecting (atrium) muscular-pumping chamber (ventricle) and an outlet pipe. There are non-return valves between the ventricle and the atrium and between

the outlet pipe and the ventricle. The valves, particularly that of the left side of the heart, are prone to disease and may have to be replaced. The outlet pipe to the left ventricle is called the aorta and the valve between the left ventricle and the aorta is known as the aortic valve. A natural aortic valve consists of three spherical leaflets connected to a common rim (stent in terminology of the prosthesis).

The geometry of the aortic valve has an important bearing on its ability to carry out its function, namely, to prevent the blood ejected into the aorta from flowing back to the left ventricle [4]. It is demonstrated in paper [5] that the dilation of the aortic root could lead to valve leakage (insufficiency), as the leaflets become too small to close the valve. In the case of irreversible, degenerative failure, the natural human aortic valve cannot work properly and must be replaced with prosthesis. There are two basic types of prosthesis of human valves [6]: mechanical and bioprosthetic ones. Compared to the mechanical valves, bioprosthetic heart valves also have successful performance and there is no need for the patient to have immuno-suppressive therapy, but their long-term performance has been disappointing. Most of the degeneration of bioprosthetic heart valves can be attributed to calcification and tearing of leaflets. The stress concentration [2] is believed to be one of the main reasons responsible for the degeneration, especially the tensile stress concentration on the opposite side of loaded surface (opposite side of loaded coating). Thus, prediction of stress distribution under loading is helpful in designing of leaflets. The scheme of the mechanical prosthesis of human aortic valve based on stress design is shown in Fig. 1a [2]. The top views of a physical model (bioprosthesis) of an aortic valve in closed and open positions, during test-

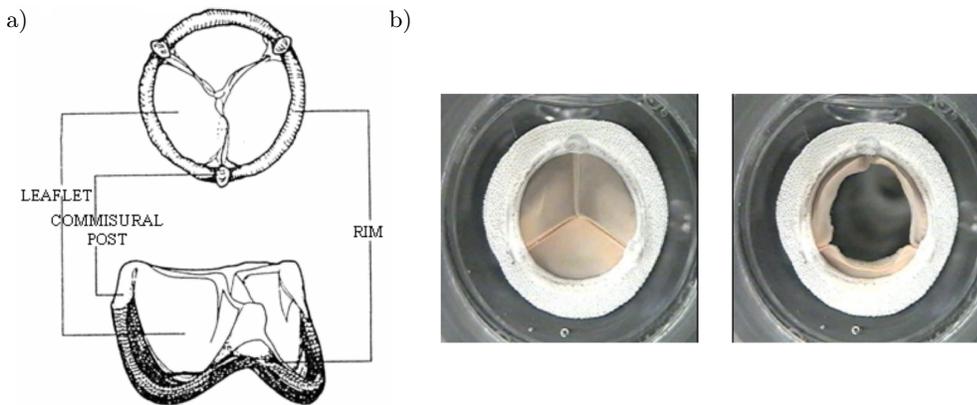


FIG. 1. a) The scheme of the prosthesis of human aortic valve [4]. b) Top views of a physical model (bioprosthesis) of an aortic valve in closed and open positions during testing in left-heart simulator [7].

ing in left-heart simulator, are presented in Fig. 1b [7]. The physical area of valve opening is calculated by comparison of the photographs of the valve in the closed and open positions [8]. The opening area is given as the parameter in the “valve’s passport”, which is prepared in experimental analysis of a valve mechanical working behaviour in the heart simulator. The calculated and registered parameters of the opening process of the valve are considered to be the most important for evaluation of the valve performance and, therefore, the physical tests are focused mainly on analyzing the opening process of the valve.

All natural aortic valves have diversified shapes and properties within a certain species and even within selected population of particular species, as it is stated for each organ, tissue etc. The Authors of the present paper examined geometry of several sheep aortic valves with cylindrical sectors of aorta, fixed in 10% formalin. Thickness and width of each leaflet of sheep aortic valve were measured several times. It is concluded, after the carried investigations, that each sheep aortic valve has a distinct shape. Results of the performed analysis allow to conclude that the model of the leaflet of human aortic valve has to be an idealization and approximation of a leaflet of the natural one. That is why the approach to geometry of an aortic valve shown in paper [2] is considered in the present work.

### 3. Physical model of monocoating PU aortic valve

The physical model of monocoating PU tri-leaflet aortic valve was realized by REUL [2]. The design analysis was prepared to obtain the physical model, which satisfies the optimum design parameters (leaflet curvatures and thickness normalized with respect to the valve ring size – aortic radius), to effect a smooth washout, minimize leaflet stress, facilitate opening of the valve at a reasonable value of the transmembrane pressure and ensure an adequate lifetime (for a given leaflet material’s fatigue data). Two alternative optimum designs (characterized by the geometrical parameters) were developed to satisfy the design criteria of the smooth washout and the minimal leaflet stress. Then, for a specific blood-compatible valve leaflet material (Avcothane-51), the leaflet thicknesses of the two design candidates were determined to satisfy the criteria of the minimal opening pressure and the adequate lifetime. The fabrication and more than 250 million cycles of laboratory tests were performed for the optimum designs.

The main requirements for the prosthesis of human aortic valve are formulated on the basis of shortly commented Reul’s research:

- a. The shape of the valve leaflets promote the smooth washout, while at the same time when the valve closes, the leaflets must come together over

- a minimal contact surface, so that red blood cell damage between the contacting surface is minimized and so that the leaflets do not stick and offer resistance to the valve opening.
- b. The shape of the valve leaflets must involve the minimum stress in the leaflet's material.
  - c. The valve must be able to withstand cycles of loading and unloading for a lifespan  $T$  ( $T = 3.5 \times 10^8$  cycles), without the fatigue failure stress being exceeded in the leaflet.
  - d. The differential pressure (loading), which causes the leaflet of valve to open (by a buckling process, illustrated in Fig. 2), must be minimal (0.7 kPa or at most 1.3 kPa).

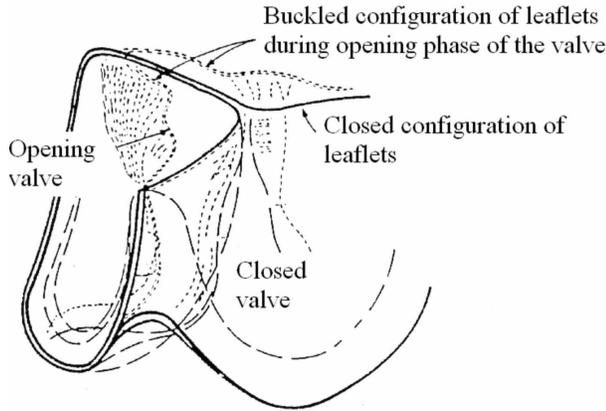


FIG. 2. Valve opening mechanism by leaflet buckling [2].

The valve opens by a buckling mode and the buckling wave travels upwards along the leaflet meridian (see Fig. 2). Hence, if the prosthetic valve is to open readily while providing minimal resistance, the value of buckling pressure is as mentioned above. By combining the equations presented in [2, 9], the critical buckling pressure  $P_b$  is expressed as:

$$(3.1) \quad P_b = \frac{32.64E}{\sqrt{1-\nu^2}} \left(\frac{d}{R}\right)^3 \left(1 - \frac{13.23}{\sqrt{1-\nu^2}} \frac{d}{R}\right),$$

where:  $E$  – Young's modulus,  $\nu$  – Poisson's ratio,  $d$  – leaflet thickness and  $R$  – aortic radius.

This useful equation (obtained on invoking the least resistance to buckling mode of valve opening) provides the value of critical buckling pressure  $P_b$  of every valve model (Reul's valve designs I and II) for a given values of: the leaflet thickness  $d$ , the aortic radius  $R$  and the material properties characterized by the Young's modulus  $E$  and the Poisson's ratio  $\nu$ .

#### 4. Numerical model of leaflet of aortic valve and limitations

The computations are performed for a model of the leaflet of human aortic valve. It is assumed that this valve has three leaflets, which are identical in size and properties according to the experimental observations. It leads to the conclusion that the geometry of the leaflet of the human aortic valve has to be an idealization and approximation of the leaflet of the natural valve. The linear elastic model of material is used for both the developed models of the leaflet of the aortic valve (the mono-coating and the three-coating). Assuming the linear elasticity for materials of coatings is a simplification, because the real material model of polyurethane is a nonlinear elastic and TiN is an elastic-plastic material. On the basis of literature and coworker's knowledge (partners in the Polish Artificial Heart Project) it is stated that it is impossible to reach the stress values in valve leaflet, which are greater than the values of stress reached in linear elastic range measured for polyurethane and TiN. Therefore, the simplification of material model leads to smaller computing time while a reasonable accuracy of simulations is maintained.

The optimization of shape of the aortic valve is based on changing the thickness of leaflet and the aortic radius for the monocoating model. The three-coating model has the optimized Young modulus and the thickness of outer coating (percentage of thickness of the outer coating in the whole constant thickness of model). The volumetric mesh elements are generated for both the developed models. Generation of the shell elements results in a shorter computing time, but in the used commercial FEM code ADINA it is impossible to create the three-coating model, in which each coating has different thickness. The main model disadvantage of the 3D FEM model, which is large number of degrees of freedom leading to the high computing time, is reduced by applying the proper boundary conditions. These conditions are set to the outer edge of the model of leaflet and additionally, they limit the motion to expected planes (in our case, the expected planes of motion are  $x$  and  $y$  planes, the  $z$  plane is forbidden, because the motion is not observed in this plane).

The Young modulus of the inner PU coating is constant and the Young modulus of the outer TiN coating is changed in the range of values of this parameter encountered in literature. Because of the meaningfully big quotient between the constant thickness of the whole model and the changed thickness of outer coating (4-th or 5-th order of magnitude), the scaling procedure of analysed numerical model is adjusted to limited possibilities of mesh generation on thin coatings by using the commercial ADINA FEM code. Due to the character of the deposition process, high values of compressive stresses (residual stress equals about 10 GPa) are observed in the outer TiN coatings deposited on polyurethane. This fact leads to a high risk of degenerative failure of these coatings, espe-

cially on polyurethane/TiN contact region. Thus, one of the main limitations of proposed FEM model is the lack of initial distribution of residual stresses in coatings, which are experimentally determined after the deposition process.

During loading of the leaflet, the minimal pressure is applied normally to the surface (in our case it is the  $x$ -plane). This load initiates the opening process of the valve. In consequence, the present study is based on steady loading conditions, mainly because of analyzing only the opening process of leaflet and limitations of mesh generation in the commercial FEM code used.

The output result of the present model is the deformed shape of leaflet, which is helpful to estimate the percentage of valve opening after loading. Due to further application of the presented approach, the results reached for the three-coating model of leaflet are qualitatively much better than the assumption of the average Young modulus for the whole three-coating model of the leaflet. Making of the latter assumption makes impossible evaluation of the influence of thickness (for the specified Young's modulus) and the Young's modulus (for the specified thickness of coating) on rigidity of the construction of valve and, in consequence, on the opening process of aortic valve.

#### 4.1. Monocoating model of leaflet of natural human aortic valve

The idea of shape of monocoating leaflet of aortic valve is based on paper [2], where the minimal stress design of the prosthesis is performed. According to the model of aortic valve proposed by Reul, the model of geometry was realized in the present work using the SolidWorks program.

Geometrical modeling of a complex structure such as the natural human aortic valve, requires simplifying assumptions to make the approach attainable. First, it is assumed that the three leaflets are identical in size and in properties, and lie at  $120^\circ$  with respect to each other in the circumferential direction of the valve. The model of leaflet of human aortic valve is characterized by the following geometrical parameters:  $d$  – leaflet thickness,  $R$  – aortic radius,  $R_L = 1.092R$  and  $e = 1.091R$ , which are presented in Fig. 3.

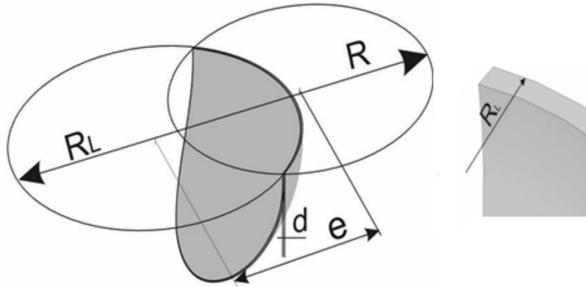


FIG. 3. The geometry of a model of monocoating leaflet of human aortic valve.

Radii and thicknesses of the leaflet of natural human aortic valve are determined by the Authors of the present work in the physiological range of values on the basis of literature research [2,10] and are as following:

- a) the leaflet thickness ( $d = 0.1\text{--}0.4$  mm),
- b) the aortic radius ( $R = 7\text{--}12$  mm).

According to the above specified values of the main geometrical parameters, the remaining parameters were calculated and they are shown in Table 1.

**Table 1. Geometrical parameters of the model of leaflet of human aortic valve [2, 10].**

Geometrical parameters, mm			
$R$	$R_L$	$e$	$d$
7	7.64	8.16	0.1
8	8.73	9.32	0.2
11	12.01	12.82	0.3
12	13.1	13.98	0.4

The material models of a leaflet of aortic valve mentioned in literature are: the Hooke model [11–14] and the hyperelastic Mooney–Rivlin or Ogden model [15]. The latter model requires many precise material constants obtained from the physical tensile strength tests. Therefore, the simplest elastic material model is used in the preliminary numerical tests. Purely linear elastic and isotropic material model is selected, which has the elastic parameters in the physiological range of values observed for natural human aortic valve and they are as indicated below:

- a) the Young modulus ( $E = 1\text{--}10$  MPa) [11],
- b) the Poisson ratio ( $\nu = 0.3\text{--}0.5$ ) [11, 12].

The loading condition is assumed as an average buckling pressure ( $P_b = 1$  kPa), which is applied as normal to the inner surface (the  $x$ -plane in the considered case). Considering the whole equation (3.1), it is obvious that for each set of parameters of the model of the leaflet of the natural human aortic valve, the critical opening pressure is different. The leaflet of aortic valve is modelled using 3D solid elements in the ADINA FEM program. Each model has 1723 nodes and 807 3D solid elements. Boundary conditions are set to the outer edge of the model of leaflet. The whole FEM model of aortic leaflet is shown in Fig. 4.

64 FEM simulations of the deformation of the leaflet of aortic valve are performed for four Young's moduli  $E(1, 2, 9$  and  $10$  MPa), thicknesses  $d$  ( $0.1, 0.2, 0.3$  and  $0.4$  mm), radii  $R(7, 8, 11$  and  $12$  mm) and Poisson's ratios ( $\nu = 0.45$ ).

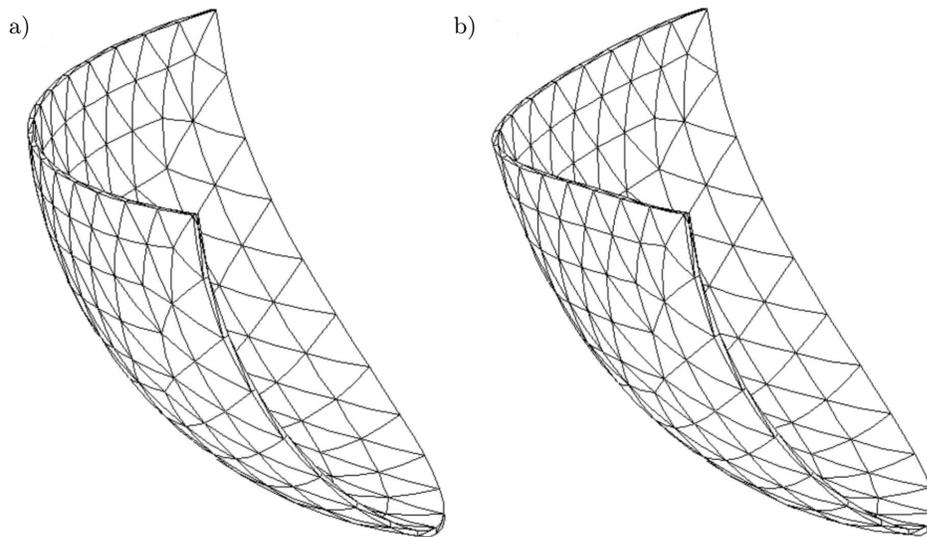


FIG. 4. The FEM model of leaflet of a natural human aortic valve: a) non-deformed (before loading), b) deformed (after loading).

Selected distributions of the effective stress expressed in pascals [Pa] and  $x$ -displacement, expressed in millimetres [mm], on inner (loaded) and outer surface of the leaflet for one version of the model, are presented in Fig. 5. The version of the FEM model, which is shown in this figure, is generated for the parameters:  $E = 10$  MPa,  $\nu = 0.45$ ,  $R = 7$  mm and  $d = 0.1$  mm. Distributions of the computed values presented in Fig. 5 show that the highest effective stress on the inner surface of the leaflet, appears in the bottom regions and near the boundary edges. The highest values of stress on the outer surface of leaflet are predicted in the bottom regions, near the boundary edges and also in the upper, central part of the leaflet. The numerical tests lead to the conclusion that advantages of the performed leaflet model of aortic valve are: the stresses have only local character and are not observed in the critical regions. The most degenerative regions of the loaded coating surface of leaflet have been determined after theoretical studies and are located on the opposite side of the loaded surface. On the contrary, the numerical investigations predict not the highest value of failure probability. Additionally, the computed values of stress in the leaflet do not exceed the linear elastic range measured experimentally for polyurethane. Therefore, the material of leaflet is not able to be nonlinearly deformed, what justifies the use of linear elastic material model.

The distribution of  $x$ -displacement is similar on both the analysed surfaces of the leaflet and the highest values of displacement are observed in the upper part of the leaflet model: in the center and near the upper boundary edges.

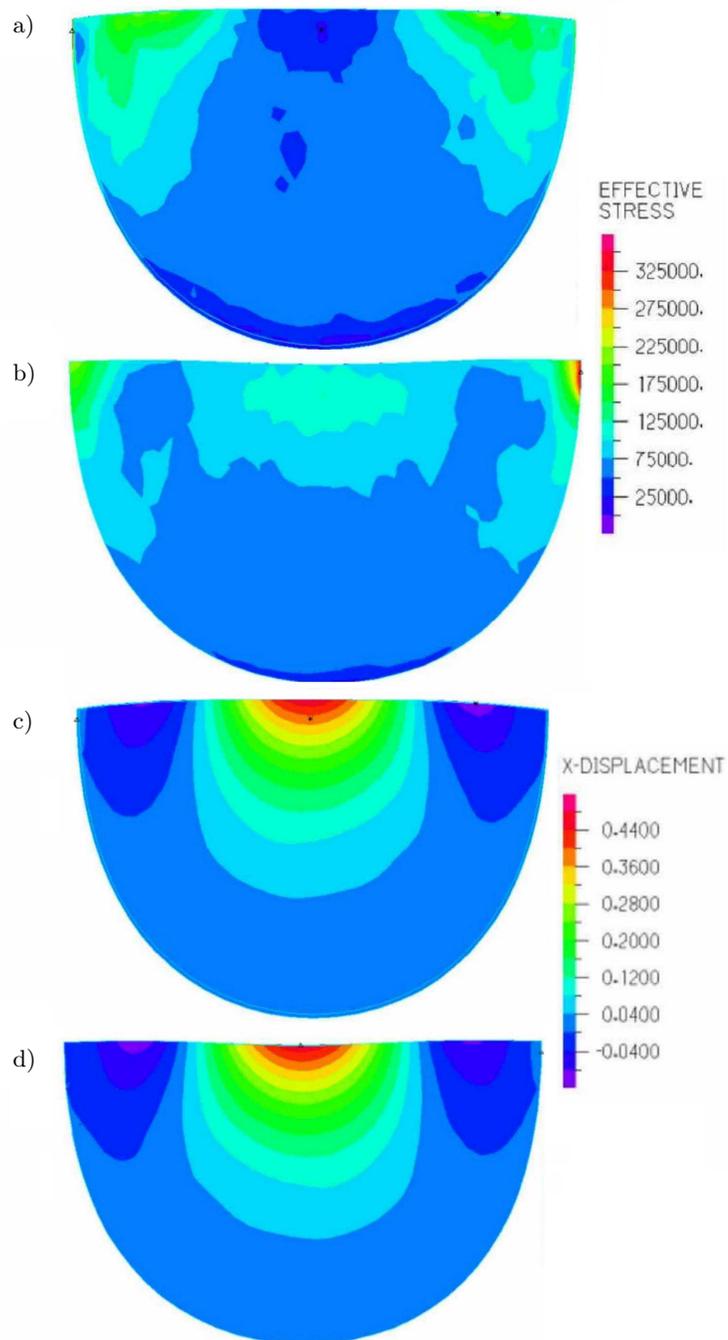


FIG. 5. Distributions of effective stress expressed in pascals [Pa] on: a) inner, b) outer surface of the model of the leaflet;  $x$  - displacement in millimetres [mm] on: c) inner, d) outer surface of the model of leaflet.

#### 4.2. Sensitivity analysis of a model of leaflet of the natural human aortic valve

Sensitivity analysis is used to determine the significant process parameters and to design the optimum values of these parameters. Moreover, sensitivity analysis specifies how and to what extent modifications of the model input data affect different change sources, and what the relationships are between the model and its input parameters [16].

The purpose of the studied analysis is to estimate influence of the selected parameter of model on the specified output. The considered input parameters of the model are: the aortic radius  $R$  and the leaflet thickness  $d$  as parameters, which describe the shape of the leaflet and the Young modulus  $E$  as a material parameter. The output of the model is defined as the maximum displacement in  $x$  direction of the node on the inner surface during loading of the buckling pressure  $P_b$  (1 kPa). The sensitivity analysis is based on the finite difference approximation. The main advantage of this method is no modification of the original model, which is completely introduced in Sec. 3.1. It should be emphasized, that this method is not the most accurate, but gives reasonably good results.

The sensitivity coefficients  $\varphi_{p_j}$  [16] are defined as:

$$(4.1) \quad \varphi_{p_j}|_{\mathbf{p}^*} := \left. \frac{p_j^*}{X(\mathbf{p}^*)} \frac{\partial X}{\partial p_j} \right|_{\mathbf{p}^*} = \frac{p_j^*}{X(\mathbf{p}^*)} \frac{X(\mathbf{p}^* + \Delta p_j \mathbf{e}_j) - X(\mathbf{p}^*)}{\Delta p_j},$$

where:  $\mathbf{p}^* = \{R^*, d^*, E^*\}$  – vector composed of the aortic radius  $R$ , the leaflet thickness  $d$  and the Young's modulus  $E$ ,  $\mathbf{e}_j$  – vector of the canonical basis,  $\Delta p$  – variation of the parameter  $p$  and  $X$  – maximum displacement.

Two points were analyzed for each parameter and are defined as lower and upper limits of the appropriate parameter. The limits of parameters are identified according to the literature research and described in Sec. 3.1. The sensitivity coefficients are calculated for each value of the parameter and for perturbed values of remaining parameters, to verify if the sensitivity coefficients are independent or not of the other parameters. The results for examined parameters of the sensitivity analysis are shown in Fig. 6.

The conclusions achieved in the presented sensitivity analysis are as indicated below:

- a. The model of leaflet of aortic valve is most sensitive to the aortic radius and between the assumed values of this parameter, the sensitivity does not vary noticeably.
- b. The model is less sensitive to the second geometrical parameter – thickness, and material parameter – the Young modulus, but sensitivity coefficients still have meaningful, large values.
- c. All analyzed parameters control the considered output of the model of leaflet and they should be taken into account in the future research. The

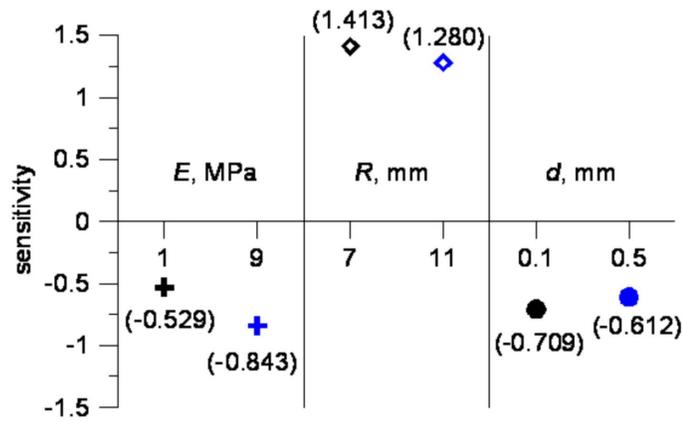


FIG. 6. The sensitivity coefficients calculated with respect to the Young modulus  $E$ , the aortic radius  $R$  and the leaflet thickness  $d$ .

biggest sensitivity coefficients are obtained for the monocoating leaflet of the aortic valve, characterized by the following values of the parameters:  $d = 0.1$  mm and  $R = 7$  mm. These geometrical parameters are set as the input parameters for the extended numerical model of a three-coating leaflet of aortic valve.

#### 4.3. TiN/PU/TiN model of leaflet of human aortic valve

The conclusions drawn from the sensitivity analysis for the model of monocoating leaflet lead to the set of geometrical input parameters of the TiN/PU/TiN model of leaflet of human aortic valve:  $R = 7$  mm and  $d = 0.1$  mm. The Young modulus of the inner coating (PU) is assumed as a constant value and equal to  $E = 10$  MPa [17]. The selected input values of geometrical and material parameters give a minimal value of the buckling pressure, which equals 0.77 kPa. This new construction of the leaflet is tested for the five geometrical ratios between the thickness of the deposited outer coating and the thickness of the whole leaflet (0.092 mm). Since the material properties of TiN depend on the type of the deposition technique and on the conditions used in the deposition process, the tested values of Young modulus in the models have very wide range from 10 MPa to 100 GPa, which are mentioned in literature [18–23].

The generated five versions of TiN/PU/TiN model of a leaflet have the following thicknesses of each coating:

- 1) 0.003 mm/0.086 mm/0.003 mm,
- 2) 0.002 mm/0.088 mm/0.002 mm,
- 3) 0.001 mm/0.09 mm/0.001 mm,
- 4) 0.0007 mm/0.0906 mm/0.0007 mm,
- 5) 0.0003 mm/0.0914 mm/0.0003 mm.

The geometry of the model of the leaflet is presented in Fig. 7. The numerical model of a three-coating leaflet of aortic valve is generated in the 3D ADINA FEM code and is composed of 11 000 elements and 10 000 nodes.

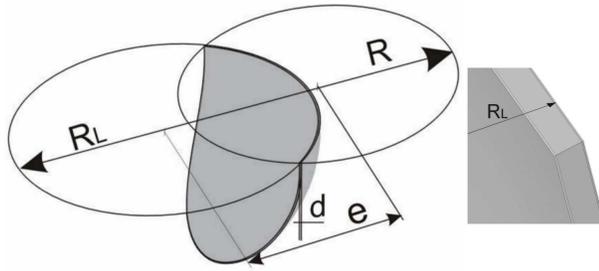


FIG. 7. Geometry of the model of the three-coating leaflet of the human aortic valve.

In the first step, the opening process of the TiN/PU/TiN model of leaflet is defined by the displacement in the  $x$  direction, which is reached in its characteristic point (the direct output parameter of the investigated model), what is shown in Fig. 8a. The displacements in the characteristic point of the leaflet for the valve opening are shown in Fig. 8b for the selected Young modulus of outer coating in the 3-rd version of FEM model.

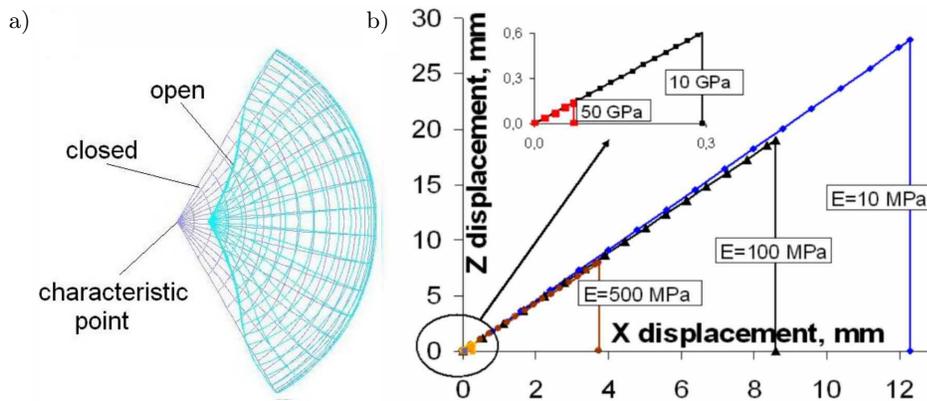


FIG. 8. a) The FEM model of three-coating leaflet of the human aortic valve in open and closed positions (top view in the  $xy$  plane), b) The valve opening for selected Young moduli in the 3-rd version of the model.

Assuming such the valve opening process and the  $x$  displacement as the output of the FEM model, the sensitivity coefficients (Eq. (4.1)) for this parameter with respect to the Young modulus of outer coating are calculated for the 3-rd version of the model and plotted in Fig. 9.

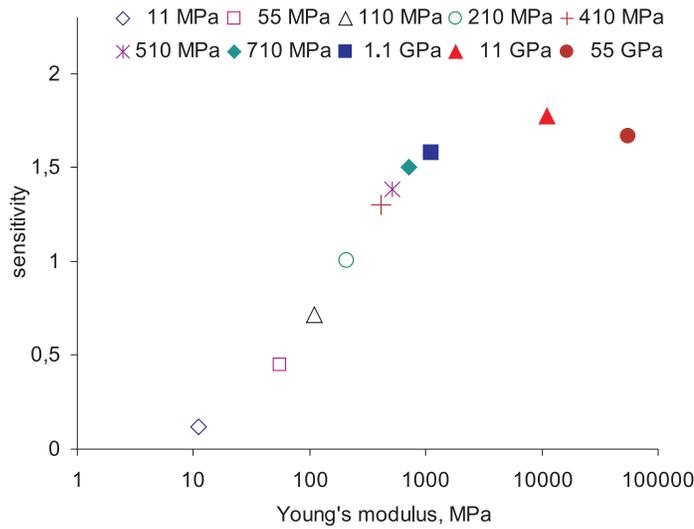


FIG. 9. The sensitivity coefficients with respect to the Young's modulus for the 3-rd version of the model.

Following these results, further calculations are carried out for the remaining versions of the model of the leaflet and, especially for the Young modulus, which corresponds to the great value of the sensitivity coefficients for the 3-rd version of the model. Thus, the computational cost of simulations is smaller, because fewer simulations are necessary for the remaining four versions of the model.

The displacement leaflet opening (*DLO*) for the set of values of the Young modulus in all the created versions of the FEM model is shown in Fig. 10. This

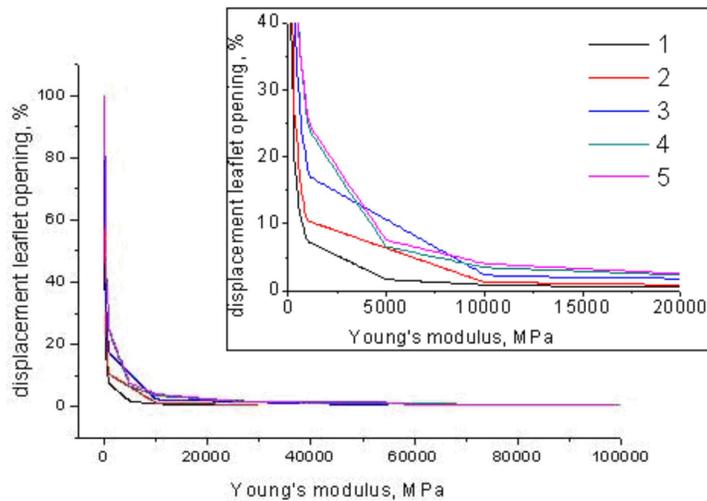


FIG. 10. The displacement leaflet opening versus the Young's modulus for five versions of the model.

opening is calculated according to the following formula:

$$(4.2) \quad DLO = \frac{(D_{E_I=E_E} \cdot 100\%)}{D_{E_I \neq E_E}},$$

where:  $D_{E_I=E_E}$  – the displacement of the leaflet composed of three coatings, which have the same Young moduli,  $E_I$  – the Young modulus of the inner coating,  $E_E$  – the Young moduli of the outer coating and  $D_{E_I \neq E_E}$  – the displacement of the leaflet composed of three coatings, which have different Young moduli of inner and outer coatings.

The thicker is the outer coating, the smaller will be the displacement leaflet opening  $DLO$  for the same value of the Young modulus of compared versions of the model. It is found that for the Young modulus greater than 30 GPa, the leaflet is closed in all the cases examined.

In the second step, the opening process of the TiN/PU/TiN model of the leaflet is defined by the area of opening calculated by comparison of the meshes before and after the loading (buckling pressure) in the AutoCad program. This approach to estimate the opening process is based on the experimental procedure, which is dedicated to the analysis of valve photographs made in open and closed positions during testing of the physical models in the heart simulator [7, 8] and after calculations presented in the “valve’s passport”. The examples of investigated images of meshes generated in the ADINA FEM code for each simulation are shown in Fig. 11. The results of selected simulations of the leaflet during opening in the 5-th version of the model of the leaflet for the Young modulus 10 MPa, 500 MPa, 5 GPa and 25 GPa are demonstrated in this figure.

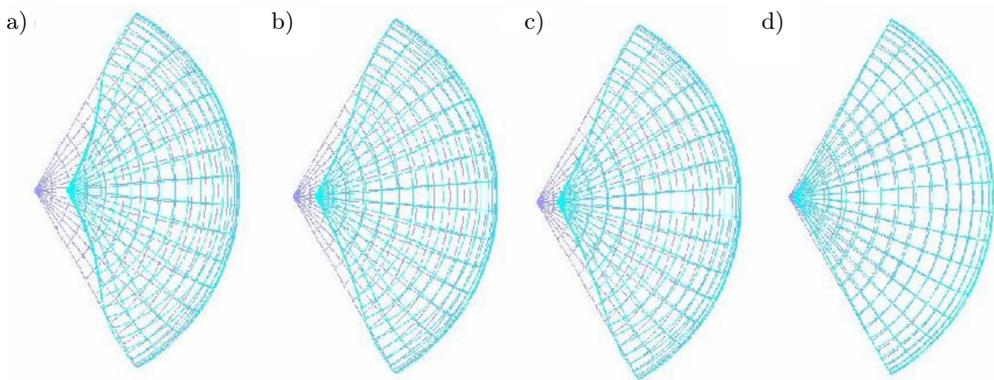


FIG. 11. The FEM meshes during opening in the 5-th version of model of leaflet for the Young's moduli (top view in the  $xy$  plane): a) 10 MPa, b) 500 MPa, c) 5 GPa and d) 25 GPa.

The results of area leaflet opening for the complete set of Young’s modulus in five versions of the model of the leaflet are presented in Fig. 12. The plotted area leaflet opening  $ALO$  is calculated according to the equation:

$$(4.3) \quad ALO = \frac{(R_{L_c}^2 - R_{L_o}^2) \cdot 100\%}{R_{L_c}^2},$$

where:  $R_{L_c}$  – radius  $R_L$  of a closed leaflet,  $R_{L_o}$  – radius  $R_L$  of an open leaflet,  $R_L$  – radius calculated in Table 1 and defined in Sec. 3.1.

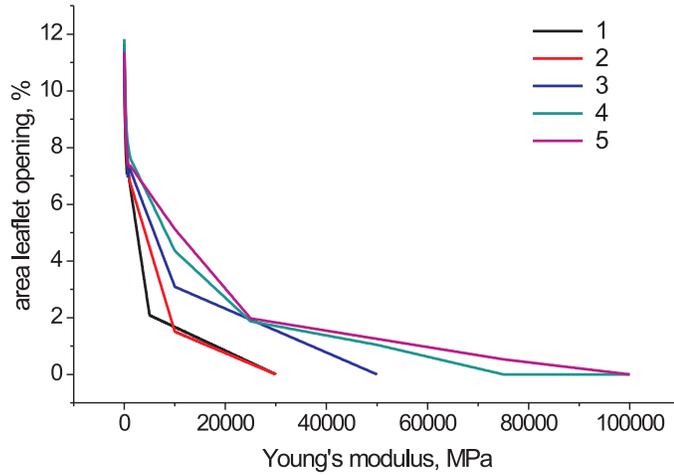


FIG. 12. The area leaflet opening versus the Young’s modulus in five versions of the model.

The character of curves shown in Fig. 12 is similar to the graphs demonstrated in Fig. 11. The results, which are used to draw the plots in Fig. 12, present more visible differences between the examined versions of the leaflet model. The greatest difference is observed between the versions of model with the thickest (1-st version) and the thinnest (5-th version) outer coating. To summarize, the thicker is the outer coating, the smaller will be the area leaflet opening and the thicker is the outer coating, the smaller will be the Young modulus required to reach the closed position of the leaflet. It is observed that each version of model closes for different values of the Young modulus. It is generalized that the thick versions of the model (1-st and 2-nd) close for the same value of the Young modulus, and the thin versions of the model (5-th and 6-th) also close for the same value of the Young modulus. The 3-rd version of the model closes independently for the value of the Young modulus located at the midpoint of thick and thin models. Small values of the Young modulus of the outer coating do not introduce any noticeable differences between the models, what is

manifested by overlapping the curves obtained for each model. This statement is true for both methods (displacement and area leaflet opening: *DLO* and *ALO*) of estimating the leaflet opening process.

## 5. Conclusions and discussion of results

The sensitivity analysis with respect to the particular parameter is performed for the monocoating model of leaflet of natural human aortic valve. The examined parameters of the model are: the Young modulus, the aortic radius and thickness of the leaflet. The results obtained from the sensitivity analysis for the monocoating model of leaflet are used as the input data for the three-coating model of leaflet of human aortic valve.

Several versions of three-coating model of leaflet of human aortic valve with different thickness of outer coating are presented in the paper. It is assumed that the whole thickness of the model of the leaflet is equal to 0.092 mm, what corresponds to the thickness of a selected leaflet of natural human aortic valve. According to the achieved results of FEM simulations, it is stated that:

- a. The greater is the value of the Young modulus, the greater will be the sensitivity of model of leaflet with respect to this parameter. The biggest sensitivity is observed for the largest Young modulus considered  $E = 11$  GPa.
- b. The opening process of the leaflet of the aortic valve is analysed by using two methods of measurement:
  - the displacement of leaflet opening (*DLO*),
  - the area of leaflet opening (*ALO*).

The Authors made an assumption that 1% opening of the leaflet is considered as the initiation of the valve opening process and, therefore, the following conclusions are drawn:

On the basis of the method related to the measurement of the area leaflet opening:

- The model of leaflet is very rigid and the thickness of the outer coating does not influence the valve opening process for the 1-st and 2-nd versions of the model. The value of the Young modulus, which initiates the opening process of a valve (critical value), is equal to 20 GPa for both the mentioned versions of the model.
- The thinner is the outer coating, the greater is the critical Young modulus. It is observed that small change of percentage of the thickness of the outer coating involves large perturbation of the Young modulus. Considering Fig. 12 (4-th and 5-th versions of model), the increment of the Young modulus is small, what is caused by the too thin outer coating. Such thin coating does not have any effect on the rigidity of the whole model.

- There is no meaningful influence of the thickness of the outer coating on the initiation of the opening process of valve for the smallest values of the Young modulus (10 MPa–4000 MPa).
- Influence of the thickness of the outer coating on the initiation of opening process of valve is visible, if the quotient between the Young modulus of outer coating and the Young modulus of inner coating is equal to 5 or is greater than this value. The greater is the described quotient, the more meaningful is the mentioned influence.
- The highest sensitivity with respect to the change of Young modulus is observed for 11 GPa, what is also confirmed by the results of the sensitivity analysis presented in Fig. 9.

On the basis of the method related to measurement of the displacement leaflet opening:

- When the Young modulus is greater than 20 GPa, the displacement at a characteristic point does not appear in the specified direction (the  $x$  axis) for all versions of the model of the leaflet.
- The model of the leaflet moves in two directions and, therefore, the displacement of characteristic point should be also analysed in the perpendicular axis (the  $y$  axis), what is realized by using the second method of measurement, which is the area leaflet opening.

The results shown in the paper lead to a general conclusion that the proper work of the TiN/PU/TiN model of human aortic valve for the greatest predicted value of the Young modulus obtained in deposition process of TiN coating on PU substrate is satisfied, if the thickness of the outer coating is less than 0.0003 mm. It is valid for the assumption that the thickness of the deposited coating is less than 1% of the whole thickness of the leaflet.

The Young modulus for the thickest outer coatings, which satisfies the proper work of aortic valve, should be smaller than 20 GPa.

The numerical tests lead also to the conclusion that the advantages of the model of the aortic valve leaflet are: the stresses have only a local character and are observed in the bottom regions of the leaflet, near the boundary edges and in the upper part of the leaflet. They are not observed in the critical regions (opposite side of the surface). The results of the investigations decide about not the highest value of failure probability. But the best and complete future model of synthetic aortic valve should consider the distribution of initial residual stresses, which are experimentally measured after the deposition process.

Additionally, the computed values of stresses in the leaflet do not exceed the elasticity limit measured experimentally for polyurethane and TiN. Therefore, the material of leaflet is not subjected to nonlinear and/or plastic irreversible deformation, what is usually responsible for the leaflet failure. Thus, assuming linear elastic models for both the valve materials (PU and TiN) is justified.

## 6. Summary and prospects

The numerical project of three-coating leaflet of human aortic valve composed of three identical leaflets developed presented in the paper, is realized in the following stages:

1. The analysis of physical Reul model, which was performed for the mono-coating synthetic aortic valve, in order to determine and further to satisfy the main criteria of proper work of the aortic valve, such as minimal buckling pressure and minimal stress in the leaflet during the valve opening process.
2. Development of the numerical model of monocoating leaflet of natural human aortic valve, which is based on the literature research and Reul physical equations.
3. The sensitivity analysis of the model of monocoating leaflet of natural human aortic valve, which is used to obtain the values of geometrical parameters. These parameters are further the input settings of the model of three-coating leaflet.
4. Creation of the model of the three-coating leaflet of the human aortic valve, with different thickness and Young modulus of the outer coating.
5. Elaboration of the two methods of estimating the valve opening process in the numerical model of the three-coating leaflet of the human aortic valve.
6. Application of the sensitivity analysis to specify the influence of material properties of the outer coating on the response of the model of the three-coating leaflet, what is considered in further investigation and cuts down the computing time.

The proposed approach to the studied problem (the valve opening process) leads to prepare the project of the TiN/PU/TiN model of human aortic valve composed of the three identical leaflets, which fulfils the assumed criteria. The type of deposition technique and conditions of the deposition process should be correctly reproduced for outer coating (TiN) in the future, to obtain the required material properties, what will enable proper work of the aortic valve considered as minimal buckling pressures and minimal stress in the leaflet during the opening process. This effect is crucial for the sake of the long-term work of aortic valve.

The real pressure, which fully opens the natural human aortic valves in the circulatory system, is ten times higher than the minimal buckling pressure considered as the loading of model of leaflet in the present paper. Due to this, even the examined valve with a thick outer coating and large Young modulus is able to open. But there is an additional satisfied criterion for the human aortic valve, which is also very important – the necessity of failure-free long-term work.

The last condition is realized only if the minimal buckling pressure and minimal stress in the leaflet of the human aortic valve are reached.

The main advantage of the presented solution is the possibility to estimate precisely the opening process for geometrical and material parameters of the leaflet of the human aortic valve at the stage of designing of the model. Additionally, several problems connected with scaling of the model and generation of the FEM meshes of the model of the leaflet were overcome. These difficulties were indicated at the beginning of the present work and they decide mainly on the computing costs and accuracy of calculations.

The extension of the developed optimal aortic valve model can lead to more precise information concerning the aortic valve and will be realized by reducing the limitations of the present model, as well as by overcoming those problems, which have not been solved yet. The following steps will be realized in the nearest future:

1. Numerical analysis of the closing process and coaptation properties of the leaflets, which will be performed after generation of hybrid meshes (also hp adapted meshes) in the fluid-solid contact area.
2. Introduction of the distribution of initial residual stresses into FEM model of leaflet, which were previously experimentally measured in deposited TiN coatings.
3. Performing the unsteady simulation with physiological pressure variations over a full cardiac cycle, which should provide more faithful information about the fatigue resistance of the valve.
4. Implementation the complete material models of each coating, because of fatigue investigations (shear stress analysis) of valve materials (Point 3).

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