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Shape optimisation of a ventricular assist device using a VADFEM computer program

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The Polish ventricular assist device, POLVAD_EXT, is made of a polymer designed to be covered with a nanocoating of titanium nitride to improve haemocompatibility. A loss of cohesion can occur between the coating and the substrate. An analysis of stress and strain states in a multi-scale model of the blood chamber was performed in the finite element computer program, VADFEM. The multi-scale model is composed of a macro model of the blood chamber and a micro model of the titanium nitride (TiN) deposited on the polymer. The finite element method and the goal function, based on the triaxiality factor, are used to solve the problems formulated. The theories of non-linear elasticity and elasto-plasticity are applied. The goal of the paper is to optimise the construction of the POLVAD_EXT with respect to shape parameters.

Key words: *ventricular assist device (VAD), finite element method (FEM), optimisation, goal function, multi-scale modelling*

1. Introduction

In the literature, there are examples of multi-objective optimisation of mechanical constructions obtained by applying FEM (finite element method) simulations and optimisation algorithms with defined goal functions [1]. Multi-objective optimisation for a complex mechanical structure, the third flex arm of a manipulator in a hybrid mode aerial working vehicle, was performed in [2] by applying commercial FEM-optimisation software (Ansys). The objective was to extend the working range of the optimised element and to reduce mass by optimising geometric dimensions with the constraint of retaining strength. The algorithms were synthesised to achieve the optimal solutions as follows: a classical, gradient-based algorithm – NLPQL (Nonlinear Programming by Quadratic approximation of the Lagrangian) [3] and an evolutionary algorithm – NSGA II (Non-dominated Sorting Genetic Algorithm) [4]. This integrated method of multi-objective optimisation successfully solved the mechanical problem. Compared with enumerative methods, the efficiency was greatly improved. A multi-objective, multi-disciplinary coronary stent design optimisation paradigm was shown in [5]. The performance of the stent design is measured by the metrics of acute recoil, tissue stresses, haemodynamic disturbance, drug delivery, uniformity of drug distribution and flexibility. These metrics are obtained from computational simulations by applying the commercial software Abaqus and Star-CCM+. Design improvement is obtained using a multi-objective surrogate modelling approach, incorporating an NSGA II algorithm to search for an optimal family of designs. This methodology is useful in the development of a family of stents with increased resistance to in-stent restenosis and thrombosis. In summary, the presented approaches to developing complex mechanical and biomedical constructions on a macro-scale were successfully realised using commercial, FEM-optimisation software.

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The next biomedical construction that needs optimisation is the Polish pneumatic ventricular assist device [6], POLVAD_EXT, which was developed by the Polish Artificial Heart Program. The POLVAD_EXT is composed of a blood chamber and two connectors (Fig. 1). The blood chamber works under cyclic loading. The walls of the VAD are composed of a temperature-sensitive polymer, ChronoFlex C 55D, and are covered with a nanocoating of titanium nitride (TiN), applied by laser ablation, to improve haemocompatibility in [7]. The blood chamber is designed to have a multi-layered structure. Thus, any fractures between the coatings and the substrate can be observed. A detailed analysis of stress and strain states, on both micro and macro scales, is needed. The Polish proposition of the construction of a pneumatic ventricular device is similar to the constructions of Abiomed AB5000 (USA), Thoratec PVAD (USA), Berlin Heart EXCOR (Germany) and Medos HIA-VAD (Germany). The VADs listed in [8] are not coated. The Polish construction of the VAD is nearest in design to the construction of Medos. Work published on the VADs listed has been dedicated to blood flow characteristics on both macro [9] and micro scales [10], [11]. In summary, there is a lack of physical and numerical models in the literature that have a multi-layer construction like that of the POLVAD_EXT. Thus, the literature review dedicated to multi-scale modelling of the POLVAD_EXT is primarily based on the work performed by the contractors of the Polish Artificial Heart Programme who developed the device.

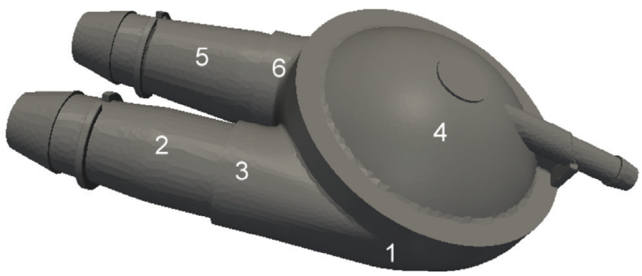

Fig. 1. CAD model of the POLVAD_EXT:
1 – blood chamber, 2 – inlet connector, 3 – inlet valve,
4 – pneumatic chamber, 5 – outlet connector, 6 – outlet valve

The problem of linear elasticity was solved on a macro and micro scale using a finite element code, VADFEM. The macro scale model of the blood chamber and a micro-scale model of the TiN deposited on the polymer were applied during FEM simulations. In the first step, a comparative analysis of the latest construction of the VAD, the POLVAD_EXT, versus its older version, the POLVAD, was performed in [12]. Numerical comparisons of the Polish VADs show that the newer version of the blood chamber generates smaller amounts of stress and strain, minimising the possibility of fracture between the coating and the substrate. Therefore, the construction of the POLVAD_EXT is better than that of the POLVAD with respect to the stresses and strains that occur between the two connectors on the internal surface of the blood chamber. However, the strains are reached in linear elastic intervals in both versions of the VADs. In the second step, identification of the material model of TiN was investigated in [13]. The supplemented version of the micro model is composed of residual stress, material models of the substrate and the coating, stress resulting from loading of the macro model, thickness of the coating, and wave parameters of the surface of the coating (wavelength and amplitude). The influence of each parameter of the micro model on strain and stress was examined in [14]. The extended version of the micro model was investigated for both versions of the VADs, the POLVAD and the POLVAD_EXT, by applying a factor analysis. The maximum stresses and strains were concentrated between the coating and the substrate in the micro-scale models of the Polish VADs investigated, as well as at the critical points of the micro model, which are the wave nodes of the surface of the nanocoating. Smaller stresses and strains are computed in the micro model of the POLVAD_EXT. The last step of the research was dedicated to validating the non-linear FEM solution developed for a macro model of the POLVAD_EXT with digital image correlation (DIC) data (displacements and strains) obtained on the external surfaces of the blood chamber in [15]. Additionally, the relaxation iterative method of solving the non-linear boundary problem was introduced to decrease computing time in [16]. The agreement between the experimental (DIC) and numerical (FEM) results is quite good in [15], [16]. Therefore, the data computed in the macro model of the POLVAD_EXT are reliable, as validated in the proposed experiment, as well as accurate and reproducible.

Considering the robustness of the algorithms applied in the FEM software, the short computation time needed for a 3D non-linear solution, and the completeness of the multi-scale model of the POLVAD_EXT, the VADFEM computer program that was developed is expected to optimise the shape parameters of the POLVAD_EXT in the present work.

2. Materials and methods

2.1. Experiments

The experiments were performed in previous studies [13], [15] and [17]. These results represent input and validation data for the multi-scale model developed in the VADFEM computer program. Experimental tests were performed as follows:

(a) A tension test was used to identify the material model of the polymer – ChronoFlex C 55 D in [15]

$$\sigma = 104.54\varepsilon^{0.75}\exp(-3.37\varepsilon)\exp(-0.04t) \qquad (1)$$

where t is a temperature, ε is a strain, and σ is a stress.

(b) Digital image correlation was applied to determine the displacement and strain on the external surface of the VAD [15].

(c) X-ray diffraction was adopted to measure residual stress (2 GPa) in the TiN nanocoating in [17], and TEM (Transmission Electron Microscopy) images were used to determine the sinusoidal shape of the surface of the TiN nanocoating in [13] using the following parameters: thickness – 350 nm, amplitude – 50 nm, and wavelength – 350 nm.

(d) A nanoindentation test was used to identify a bilinear, elastic-plastic material model of the TiN nanocoating in [13]: ε_1 = 0.009, σ_1 = 2 614 MPa, ε_2 = 0.166, and σ_2 = 9 107 MPa.

2.2. VADFEM computer program

The VADFEM computer program that was developed allows for the modelling of strain and stress states in multi-layer ventricular assist devices, such as the POLVAD and the POLVAD_EXT. The task posed is solved on a macro [12] and a micro-scale [14]. Micro-scale modelling is helpful for evaluating the probability of a fracture between the polymer and the coating. Fractures can be caused by the stress and strain induced by the influence of loading, especially on the internal surface of the blood chamber that is coated by the TiN nanocoating. Additionally, the micro solution was used to identify the material model of the TiN in [13] and to perform a sensitivity analysis of the TiN/substrate in the nanoindentation test in [18].

The algorithms [19] were implemented in the VADFEM computer program to solve the finite element mesh processing and to implement boundary conditions. Automatic fragmentation of the FE mesh provides opportunities to calculate the macro solution in the FE mesh of the VAD that can be generated by any commercial program and allows the boundary conditions to be set in any location of the VAD. The problem of convergence in non-linear tasks (non-linear elasticity and elasto-plasticity) in a macro model of the VAD was efficiently solved by applying relaxation iterative methodology. The methodology proposed in [16] decreased by two fold the number of iterations, and therefore, the computing time was significantly reduced. Fast convergence in non-linear problems is particularly important in the VAD macro-scale model due to the large number of elements and the type of loading known as pressure loading.

The results of the VAD computed in the VADFEM software were compared with:

(a) strains and stresses reached in a commercial FEM code, Abaqus in [20], and

(b) strains and displacements obtained by digital image correlation in [15].

Thus, the numerical and experimental validation of the results of the VAD affirmed the correctness of the VADFEM computer program. The VADFEM software is used in the present work to simulate a macro model of the POLVAD_EXT and to optimise the shape parameters of the POLVAD_EXT.

2.2.1. Macro model of POLVAD_EXT

The macro model of the POLVAD_EXT is prepared in the VADFEM computer program. The macro-scale boundary problem is formulated for the theory of non-linear elasticity and a distribution of displacements, U_i. This approach describes deformation of the chamber of the POLVAD_EXT under blood pressure if stresses are related to strains by non-linear equations (according to the non-linear theory of elasticity) and if the strain disappears in unloading conditions. Non-linearity in the elastic deformation process of the blood chamber is a result of the non-linear mechanical properties of ChronoFlex C 55D and the TiN nanocoating.

On a macro-scale, the deformation of blood chamber is considered as a 3D solution. Thus, the defined boundary problem of the theory of non-linear elasticity is composed of the groups of equations described in [21]. In a non-linear zone of deformation, an effective stress, σ_i, is a function of an effective strain, ε_i, and a temperature, t. The effective modulus is used instead of Young's modulus in each iteration. The problems of convergence in a non-linear task in a macro scale are solved in the present work by the use of an iterative method. The effective modulus,

E_{eff}, is calculated in the next iteration, $k + 1$, using the following formula

$$E_{\text{eff}}^{(k+1)} = \frac{\sigma_i^{(k)}}{\varepsilon_i^{(k)}} \tag{2}$$

where $E_{\text{eff}}^{(k+1)}$ is the effective modulus in the next iteration, $\sigma_i^{(k)}$ and $\varepsilon_i^{(k)}$ are the effective stress and effective strain in the current iteration, respectively, and k is the number of iterations.

The error of the effective modulus, δ, is calculated by applying the formula

$$\delta = \frac{E_{\text{eff}}^{(k)} - E_{\text{eff}}^{(k+1)}}{E_{\text{eff}}^{(k)}} \tag{3}$$

where $E_{\text{eff}}^{(k)}$ is the effective modulus in the previous iteration and $E_{\text{eff}}^{(k+1)}$ is a value calculated using equation (2).

The relation, $\sigma_i(\varepsilon_i, t)$, is determined according to equation (1). The components of a stiffness matrix, $[K]$, and the complete load vector, $\{F\}$, are written according to the following formulas

$$[K] = \int_V [B]^T [D][B] dV , \tag{4}$$

$$\{F\} = -\int_S [N]^T \{p\} dS , \tag{5}$$

where S is a contact surface, $\{p\}$ is a pressure inside the blood chamber, $[B]$ is a matrix containing derivatives of shape functions, $[D]$ is a matrix containing appropriate material properties (E, ν), $[N]$ is a matrix of shape functions of a finite element, and V is a volume.

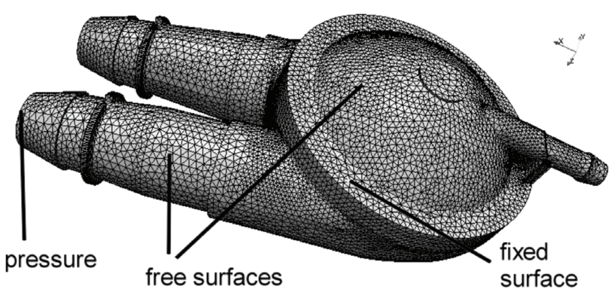

Fig. 2. Boundary conditions of the FE model of the POLVAD_EXT

A tetrahedron element with a five-point scheme of integration is used in the macro model of the POLVAD_EXT. The average number of applied nodes is 40 000 and the average number of applied tetrahedron elements is 120 000. The boundary conditions are set according to the DIC experiment [15] and are as follows (Fig. 2): (a) distribution of blood pressure, p, (37.3 kPa) on the inner surface, (b) fixed surfaces in the outer upper region (no displacement in the Z direction), and (c) unfixed surfaces in the outer region (no loading).

2.2.2. Optimisation

The multi-objective optimisation of mechanical constructions in [2] and biomedical ones in [5] using commercial software is a well-known approach that was presented in the introduction of the present work. Multi-objective optimisation of the construction of the POLVAD_EXT, by applying a VADFEM computer program, is proposed in the present paper. The objective of the present paper is the optimisation of the most important shape parameters: a thickness, h, and a distance, d, between the two connectors of the blood chamber of the POLVAD_EXT, under maximal blood pressure (37.3 kPa) and at temperature (37 °C).

The minimum of the goal function, f, was determined by the finite elements of the macro models of the POLVAD_EXT as follows

$$f = \varepsilon_i k = \varepsilon_i \frac{\sigma_0}{\sigma_i} \to \min \tag{6}$$

where k is a triaxiality factor, ε_i is an effective strain, σ_0 is a mean stress, and σ_i is an effective stress.

The selection of the goal function (equation (6)) was closely associated with the probability of damage, which can be observed in the multi-layer construction of the POLVAD_EXT when it is loaded by blood pressure. Permanent damage to the material of the POLVAD_EXT, such as fracture of the TiN nanocoating and subsequent detachment from the polymer on the internal surface of the blood chamber, can lead to obstruction. A crack may occur during plastic deformation of the TiN, which is equal to a strain of 0.009 in [13]. The examples of macro models of the POLVAD_EXT works were reversibly deformed, for instance, in [16]. The relation between stress triaxiality and stress damage due to set loading was widely described in [22]. The value of the triaxiality factor is also a criterion of selection for the group of finite elements used in the macro model of VAD, which is to be analysed on a micro-scale in the VADFEM computer program. The greatest values of the triaxiality factors are reached between the two connectors of the VAD when loaded by cyclic blood pressure, in the finite elements on the inner surface of the VAD. The selected region of the VAD macro model was further examined in the micro-scale in [23].

3. Results

The sets of CAD and FE models of the POLVAD_EXT were prepared for the purpose of optimisation. Some indispensable simplifications of the CAD model were introduced by the authors, but they did not perturb the original construction with respect to dimensions and volume. Considering the real shape of the POLVAD_EXT, the thickness, *h*, of the walls and the distance, *d*, between connectors were selected. The relationship between the goal function, effective strain, and the triaxiality factor is plotted in Fig. 3. The relationships between the goal function and the shape parameters are shown in Fig. 4. According to the results presented, the smallest goal function (f = 0.0073) was reached in model 4 (h = 4 mm and d = 15 mm), which had the largest triaxiality factor (k = 0.827) and the smallest effective strain (ε_i = 0.0088). In contrast, the largest goal function (f = 0.0092) was computed in model 5 (h = 4 mm and d = 25 mm), the model with the smallest triaxiality factor (k = 0.76) and the largest effective strain (ε_i = 0.0121). The real construction of the POLVAD_EXT was represented by model 3 (h = 3 mm and d = 25 mm), for which the goal function was quite large (f = 0.0089), as was the effective strain (ε_i = 0.0116).

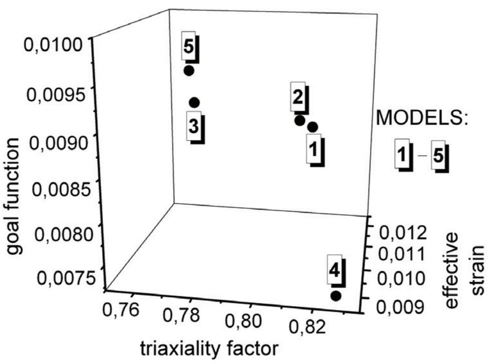

Fig. 3. Goal function versus effective strain and triaxiality factor

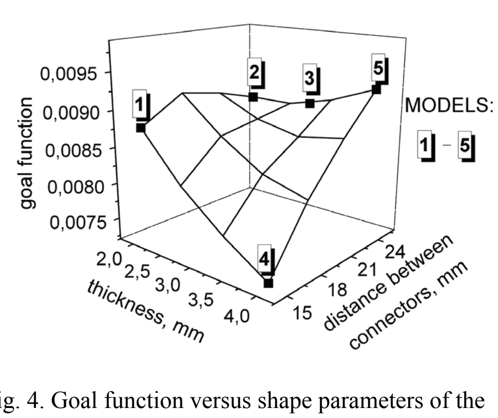

Fig. 4. Goal function versus shape parameters of the POLVAD_EXT

Effective strain proved to be the most influential component of the goal function, as the percentage change of the triaxiality factor was not very large in any of the models that were analysed. Non-linear deformation of the polymer and plastic deformation of the TiN nanocoating can be observed for an effective strain greater than 0.01. Larger deformations of the polymer and TiN lead to increased probabilities of irreversible deformation and damage to the VAD. Thus, model 4 is the best model with respect to effective strain; therefore, the smallest probability of irreversible deformation is expected for model 4. Irreversible deformation and damage are probable in model 5, making it the worst model with respect to effective strain.

4. Discussion

The analysis of results obtained by the macro models shows that the distance between the connectors is the most influential control parameter of the goal function. In conclusion, the best construction of the POLVAD_EXT with respect to the shape parameters is model 4, which has the thickest walls and the smallest distance between the two connectors. The worst construction of the POLVAD_EXT, with respect to the shape parameters, is model 5, which has the thickest walls and the largest distance between the two connectors. The real POLVAD_EXT (model 3) does not differ very much from the best mechanical construction; however, the shape parameters investigated limit the analysis to the solid solution, and the parameters examined are not the only ones to be investigated. Blood flow should be analysed in addition to fluid structure interactions (FSI). This analysis will be performed in future models developed in the VADFEM computer program.

The second step of this investigation is focused on an analysis of the local distributions of the effective strain and triaxiality factor in the real model (model 3: Fig. 5a and Fig. 6a), the best model (model 4: Fig. 5b and Fig. 6b) and the worst model (model 5: Fig. 5c and Fig. 6c) of the POLVAD_EXT. Local distributions of the parameters examined were presented on the inner surface of the blood chamber between the two connectors under a pressure of 37.3 kPa at a temperature of 37 °C. The maximum effective strain (Fig. 5) is observed in the finite elements between the two connectors. The maximum triaxiality factor (Fig. 6) is computed for the finite elements in the region closer to the centre of the two connectors.

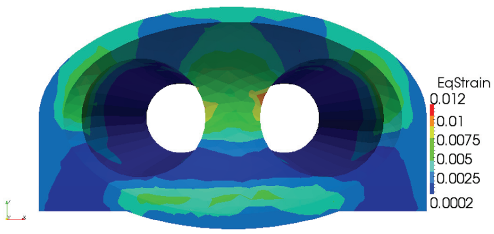

Fig. 5a. Local distribution of effective strain in model 3 of the POLVAD_EXT

Fig. 6a. Local distribution of triaxiality factor in model 3 of the POLVAD_EXT

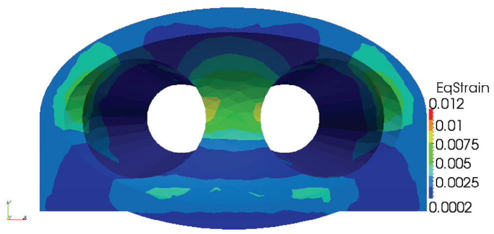

Fig. 5b. Local distribution of effective strain in model 4 of the POLVAD_EXT

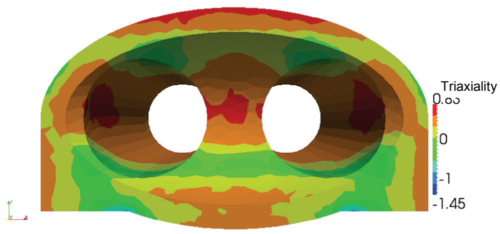

Fig. 6b. Local distribution of triaxiality factor in model 4 of the POLVAD_EXT

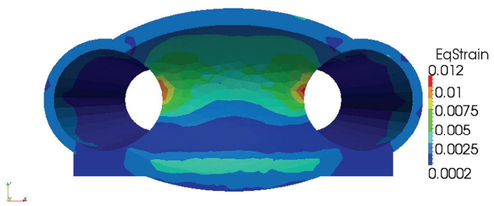

Fig. 5c. Local distribution of effective strain in model 5 of the POLVAD_EXT

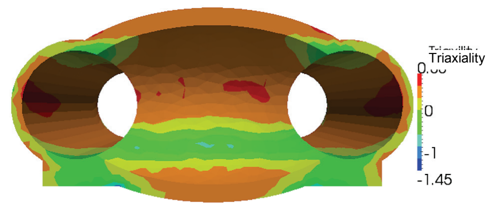

Fig. 6c. Local distribution of triaxiality factor in model 5 of the POLVAD_EXT

The optimisation parameters obtained should be incorporated in the development of future and better constructions of the POLVAD_EXT. The proposed approach is to be considered before FSI analysis. Thus, blood flow in the POLVAD_EXT will be analysed in the safest model, in which the probability of damage is significantly reduced.

Acknowledgements

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