

Grading the PVC material by solving a static inverse problem with genetic algorithm

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1. Introduction

The volumetric pump is dedicated to work for drip-feeding at hospitals. It contains the peristaltic mechanism (PM) periodically compressing so-called intro-vein set (IV-Set), which has the shape of a tube and provides a liquid into the vein of a patient. IV-Set is made up of plastic material PVC (Polyvinyl chloride).

To compress IV-Set properly, an additional simple mechanism fixing the tube is used. The fixing mechanism holds IV-Set between two plates, the lower of them is supported by several springs adjusting the plates to the tube used. The springs, in turn, should have an appropriate stiffness to compress the tube properly. If spring stiffness is too low, the tube is under-compressed, which reduces the pump efficiency. On the contrary, if the spring stiffness is too high, then the tube is over-compressed and eventually damaged.

Evidently, if neglecting the influence of friction in fixing mechanism, the total stiffness of the springs is directly proportional to the stiffness of the compressed tube, that is, to IV-Set. In turn, stiffness of the tube undergoing the deformation is subject to its geometrical shape and mechanical properties of a material the tube is made of. Thus, to calculate the tube stiffness its geometry and mechanical properties of PVC should be clear. However, the PVC grade is not provided by IV-Set manufacturer therefore the exact material mechanical properties are unknown.

The goal of this study is twofold: first, to find out mechanical properties of PVC, and second, to calculate optimal stiffness of the springs used. The optimal springs' stiffness is the one, which allows avoiding under- and over-compression of the tube in a specified temperature range. Both goals are achieved via solution of inverse problem for identification of material properties on the base of data obtained from experiment, which simulates natural behaviour of peristaltic mechanism.

The paper contains the following sections. The section *Compression experiment* presents the results of the compression experiment and provides some discussion on them. The section *Mathematical model for inverse problem* presents the problem description in mathematical terms by defining an optimization problem. The section *Identification cycle and optimization algorithms* proposes the optimization methods applied. The next-to-last section proposes a simple scheme for the computation of resultant spring stiffness. The last section draws conclusions on this study.

2. Compression experiment

The aim of compression experiment is to obtain the tube displacement/compression force curve. Only the segment of PVC tube has been investigated simulating whole peristaltic mechanism. Flat plates of fixing mechanism are replaced by the rigid contact surfaces, one of them immovable. The compression force is transmitted to the tube by movable contact surface (upper surface in our case) of the shape of mechanism's cam (Fig. 1).

We assume the vertical stiffness of the tube segment is equal (disregarding the friction influence) to the overall stiffness of spring-set on the fixing mechanism. Clearly, the inertial forces do not play significant role in mechanisms of such kind therefore quasi-static loading has been applied.

Two sample tubes in 4.10 mm in outer diameter, 3.00 mm in inner diameter, and of 200 mm length, were explored. The compression force was gradually incremented up to a certain value, which had to ensure the closure of the inner diameter of the tube. Actually the closure was estimated by visual inspection as well as by a compression curve drawn. The experiment was performed repeatedly to secure the exclusion of possible casual factors of the experiment.

The IV-Set compression test results are shown in Fig. 2, where the circle marks the region where the inner tube radius is closing. In the closing point region, the tube stiffness increases remarkably because the inner surfaces of the tube begin gaining a non-continuous surface-to-surface contact, i.e. the tube has no inner hole any longer. Actually this region is under investigation throughout the current study.

Notice, due to the insufficient cam-tube contact at the beginning of the experiment, the actual compression starts from some offset displacement value equal to 0.210 mm (see Fig. 2). Therefore, the factual displacement value at the closing point region is $3.00 + 0.210 = 3.21$ mm, which is yielded by the compressing force value equal to 10.80 N.

3. Mathematical model for inverse problem

The main idea used in identifying material properties is updating a finite element model so as to make its results converge toward the experimental results. Only the segment of PVC tube is discretized and analysed for geo-

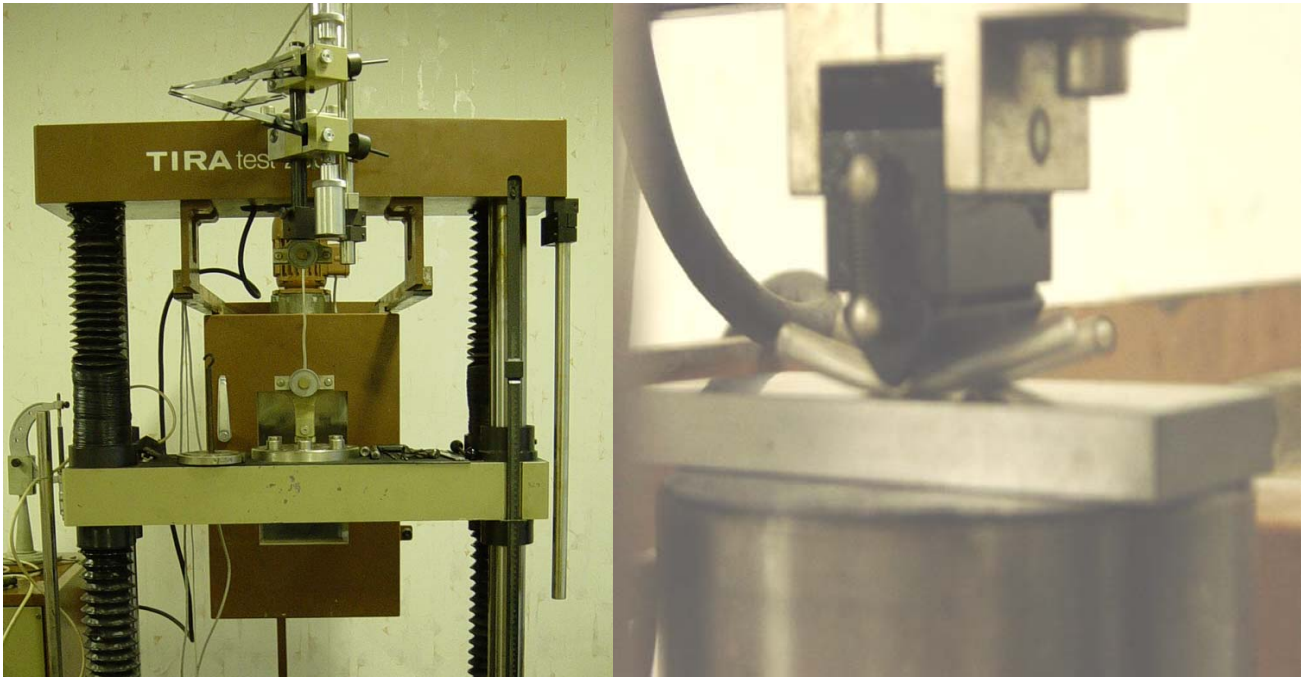


Fig. 1 Experimental set-up, and specimen under compression

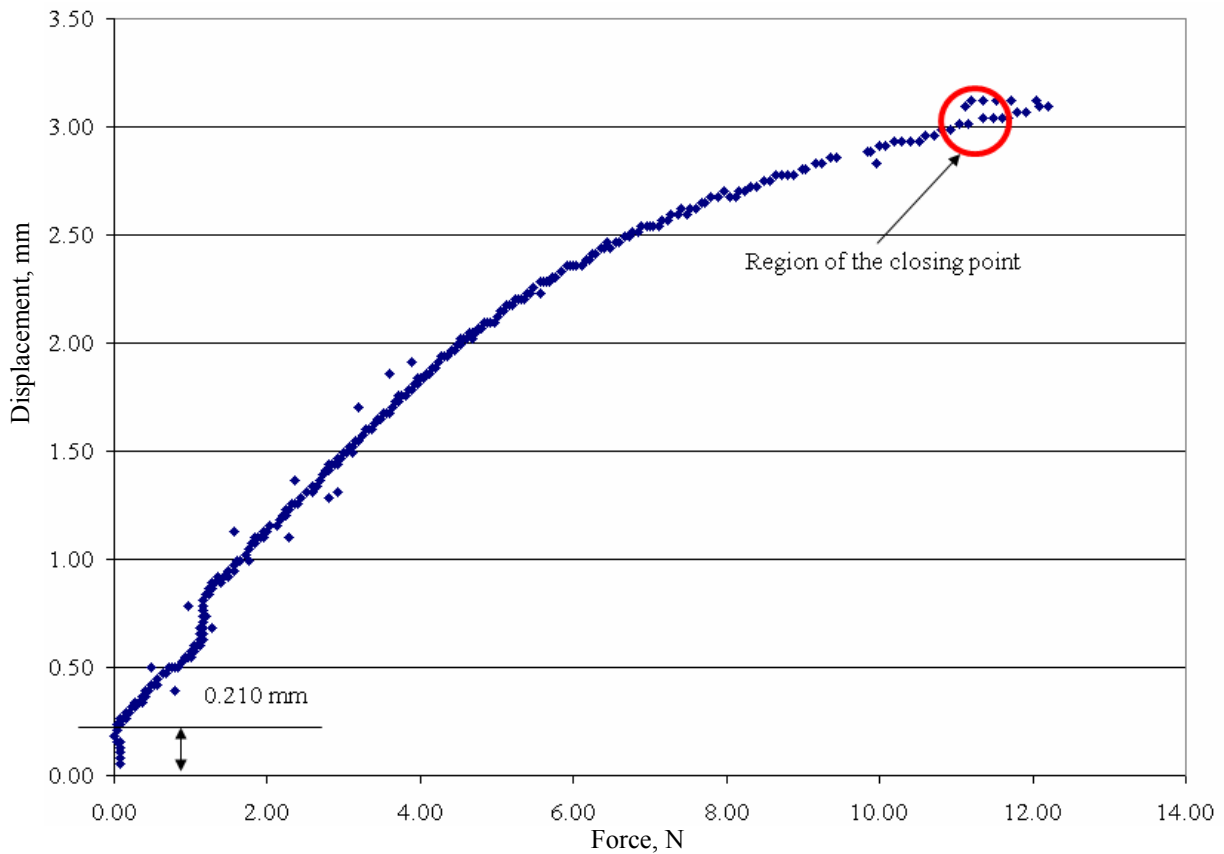


Fig. 2 Experiment results: displacement – force relation

metrically non-linear but materially linear static solution. Therefore an analysis of finite element mesh has to be done to assure the discretization errors are within acceptable range. The mesh of 3-D 10-Node Tetrahedral Structural Solid (SOLID187 in ANSYS 7.0 terms [1]) elements, which yields converged solution, is shown in Fig. 3.

The classical static equilibrium equation has the following form (1) with a non-linear stiffness matrix [2]

$$[K]\{\vec{u}\} = \{\vec{F}\} \quad (1)$$

$$[K] = [K_0(E, \nu)] + [K_s] + [K_l(\vec{u})] \quad (2)$$

where $\{\vec{u}\}$ is displacement vector; $\{\vec{F}\}$ is external force vector; $[K]$ is non-linear stiffness matrix; $[K_0(E, \nu)]$ is linear stiffness matrix, dependent on geometry of structure, material characteristics and interpolation law of finite elements; $[K_s]$ is geometrical stiffness matrix, which defines the stress influence on the stiffness; $[K_l(\vec{u})]$ is matrix of initial displacements, which defines the displacement influence on the stiffness; E is Young's modulus or tensile modulus, which is unknown; ν is Poisson's ratio.

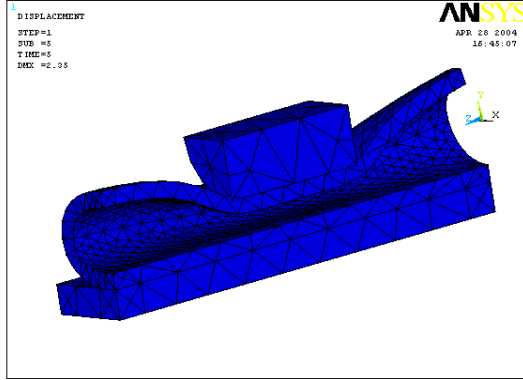


Fig. 3 Mesh of structure for converged solution

PVC is a flexible isotropic material that is chemically non reactive. Variance of Poisson's ratio among PVC grades falls into the range from 0.37 to 0.46 [3]. The variation of Young's modulus due to operating temperature range is very small and can be neglected, thus the range of interest for modulus is from 1.000 MPa to 100.0 MPa [3]. Bearing in mind that we are interested exclusively in final stiffness of the tube, which corresponds to the full closure of the tube, we arrive to two unknowns in equation (1), i.e. $[K] = [K(E, \nu)]$. Here the value of E to be sought can be interpreted as an averaged (through the whole deformation history) tensile modulus.

Now let us rewrite equation (1) in the following form

$$[K(E, \nu)]\{\vec{u}\} - \{\vec{F}\} = 0 \quad (3)$$

The last equation is suitable for the formulation of inverse problem, i.e. find material mechanical properties of the tube under known compression forces yielding a particular tube deformation, to satisfy the equilibrium Eq. (3). The formulated inverse problem can be treated as an optimization problem mathematically expressed as the following

$$\min_{E, \nu} (Q = [K(E, \nu)]\{\vec{u}\} - \{\vec{F}\}) \quad (4)$$

$$\max(\{\vec{u}\}) - d < 0 \quad (5)$$

$$E \in [E_{min}, E_{max}] \quad (6)$$

$$\nu \in [\nu_{min}, \nu_{max}] \quad (7)$$

where: Q is the objective function (OF) to be optimized; d is the displacement value at the closing point region (3.00 mm, see Section 1); (5) is the inequality constraint to be satisfied; (6) - the definition of the feasible range for tensile modulus, where E_{min} and E_{max} are lower and upper value limits respectively; (7) is the definition of the feasible range for Poisson's ratio, where ν_{min} and ν_{max} are lower and upper value limits respectively.

The next section presents the methods used to minimize the objective function (4) subject to the constraints (5-7).

4. Identification cycle and optimization algorithms

The identification cycle (Fig. 4) consists of the five parts, that is: optimization *Algorithm*, FEM modelling by ANSYS, *Fitness evaluation*, *Stopping criteria checking*, and *Printing of results*.

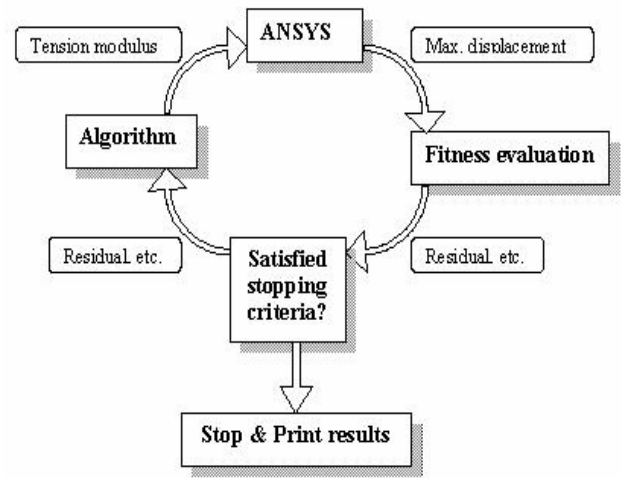


Fig. 4 Solution loop of inverse identification problem

The algorithm starts at *Algorithm* with an initial guess of tensile modulus. The *Algorithm* stands for a particular optimization algorithm, which takes an evaluated fitness value as an input parameter. Then a new guess for tensile modulus is calculated and written to ANSYS input file. The response goes from the FEM analysis. *Fitness evaluation* part compares the analysis results and experimental data. The fitness evaluation reflects the algorithm employed. If the evaluated fitness satisfies the stopping criteria, the optimization cycle stops running and results are printed. Otherwise, the results of fitness evaluation (results depend on algorithm used and may be rendered in the form of residuals, etc) are transferred back to the *Algorithm* part for further decisions.

This algorithm is common for all the optimization algorithms used. However, the fitness evaluation depends on the particular algorithm and will be presented later. The objective function Q Eq. (4) due to non-linearity of the stiffness matrix $[K]$ has uncertain landscape though the presence of the only two design parameters simplifies the solution.

To investigate the objective function landscape and solve the optimization problem defined in previous section a *Genetic algorithm* (GA) [4 - 6] as a global optimization method was employed. GA is a stochastic search method, which proved to be very convenient when OF is of

uncertain character and supposed to be non-convex, multi-modal, and discontinuous. Algorithm starts the search from an initial random guess belonging to the feasible set. This vector of initial values of design parameters is known as a *population* [4]. Later GA generates a new population at each iteration by means of genetic operators and selection mechanism. The new population is based on the previous one, however it is supposed to be fitter, i.e. closer to an optimal solution.

The algorithm has several control parameters and takes *fitness function* [4] to be optimized. The Table 1 below shows the list of control parameters, in GA notation [4].

Table 1

GA tuning parameters

Population size	20
Chromosome size	16
Probability of crossover	0.8
Probability of mutation	0.4
Relative rate for bit-flip mutation	0.5
Relative rate for one point crossover	1
Tournament size	10

The chromosome is encoded as a vector of binary numbers, which length is equal to 16, i.e. we reserved 8 bits for the tensile modulus and Poisson's ratio respectively. To decode from the genotype space to phenotype, i.e. from a binary to real number the linear mapping is used [7]

$$R(\varphi_i^k) = l + B^{-1}(\varphi_i^k) \times \frac{u-l}{2^d - 1} \quad (8)$$

where $R(\varphi_i^k)$ is a real value bounded by a predetermined interval $[l, u]$; φ_i^k is binary chromosome i at population k and d is the number of bits (we use $d = 8$); $B^{-1}(\varphi_i^k)$ denotes the mapping function from binary string to its corresponding integer [5]. We used the following real value bounding intervals for tensile modulus $E \in [1.000, 100.0]$ in MPa dimension, and Poisson's ratio $\nu \in [0.370, 0.460]$ [3]. Probabilities for genetic operators were chosen intuitively.

Fitness function takes the form, [8]

$$D(\varphi_i^k) = \begin{cases} 0 & : |s - s_{want}| < s \\ 1 - e^{-\frac{(|s(\varphi_i^k) - s_{want}| - s)^2}{2\sigma^2}} & : |s - s_{want}| \geq s \end{cases} \quad (9)$$

where $D(\varphi_i^k)$ is fitness function; $s(\varphi_i^k)$ is maximum displacement of movable contact surface at each iteration; S_{want} is target displacement value (3.21 mm, see Section 1); s is acceptance region, i.e. the tolerance value (see Fig. 5); σ is decay coefficient, which determines how fast the penalty value increases when the acceptance region is left as can be seen in the Fig. 5.

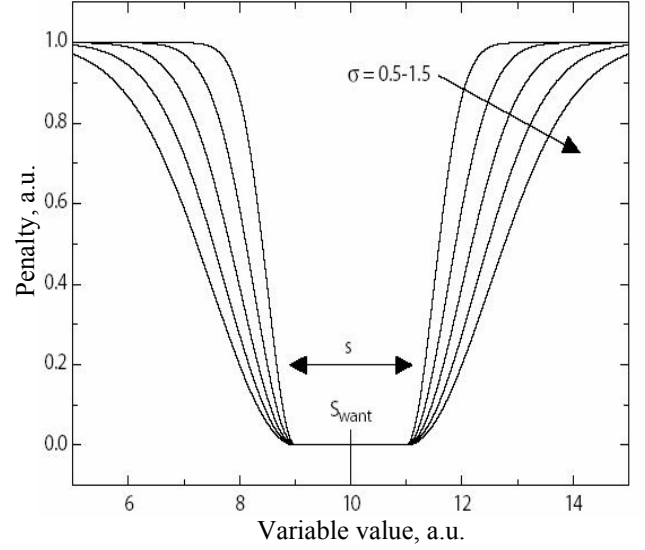


Fig. 5 Relation of decay coefficient and penalty (adopted from [8])

The Evolutionary Computation Framework (EO) [9] was employed to perform the computation.

5. Computational results

The convergence behaviour GA and landscape of OF are shown in Figs. 6 and 7 respectively.

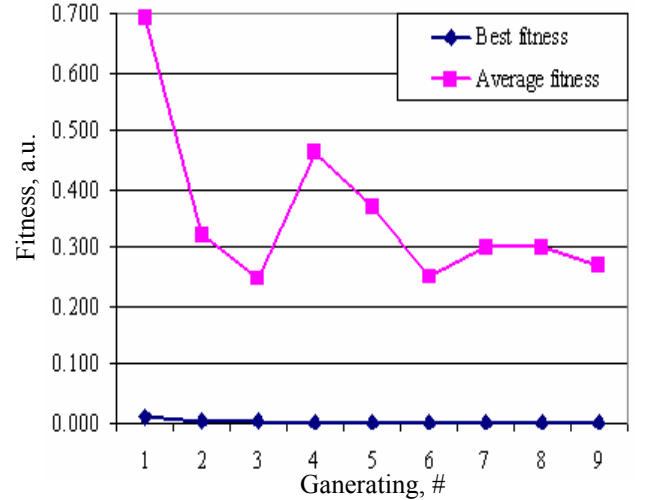


Fig. 6 GA convergence

As it is seen from Fig. 6, GA evaluated 9 generations and reached the fitness value equal to 0, i.e. the displacement value got into the acceptance region (8). Results of GA are rendered in the Table 2.

Table 2

GA optimization results

Number of evaluations/iterations	180
Number of generations	9
Tensile modulus value, MPa	9.54
Poisson's ratio	0.42
Objective function (fitness) value	0

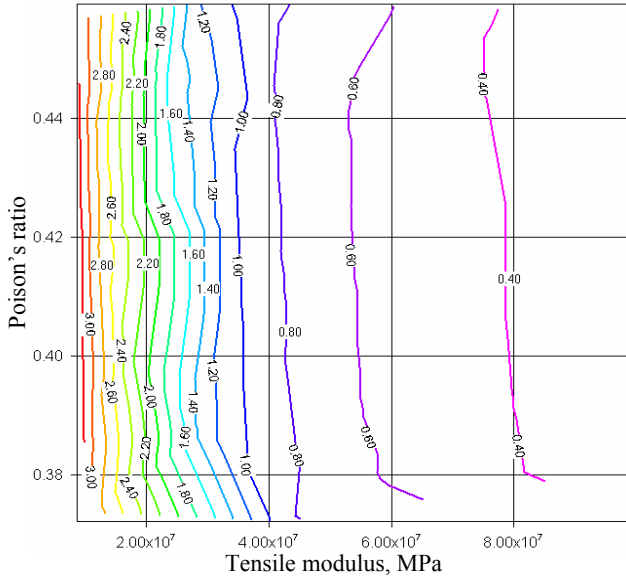


Fig. 7 Objective function landscape, where isolines show tube displacement values in mm

6. Optimal spring stiffness

Having calculated the tensile modulus and Poisson's ratio of PVC in previous sections, we could proceed in finding optimal stiffness value of the springs. The optimal spring stiffness is the one, which allows avoiding the under- and over-compression of the tube. One should notice the compressed tube stiffness is that, which turns out when closing point region (see Fig. 2) has already been reached and the tube is undergoing further compression (see Fig. 7).

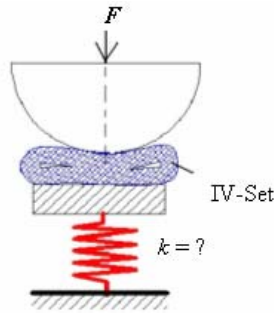


Fig. 8 Explicit tube compression scheme

If neglecting the influence of friction in fixing mechanism, resultant stiffness of the springs is directly proportional to the stiffness of compressed tube. The stiffness of compressed tube is significantly higher than its stiffness before the closing point therefore the springs start working only when the tube is compressed. Thus, a simple scheme for finding the resultant spring stiffness is considered (Fig. 8).

Simplified mathematical model of PM is shown in Fig. 9, a, where $k_i(x_i)$ denotes stiffness of the compressed tube; the tube displacement x_i varies from 0.0 mm to the closing point displacement x_c (3.00 mm), and $k_s > k_i(x_i)$ until $x_i < x_c$ - the springs' stiffness. Thus, the model of PM for the displacement level corresponding to the closing point becomes even simpler (Fig. 9, b), and the resultant spring stiffness is calculated simply dividing the force by the tube displacement value at the closing point region

(3.00 + 0.210 = 3.21 mm, see Section 2). Therefore, the resultant spring stiffness is $k = \frac{5.40}{3.21 \cdot 10^{-3}} = 1682, \text{ N/m}$.

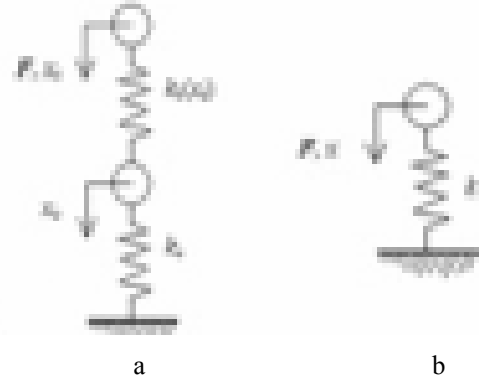


Fig. 9 Compressed tube: a) mathematical model, b) reduced mathematical model

Notice that the force value is half of the one got from the experiment (see Fig. 2). That is because we used two sample tubes in the compression test.

7. Conclusions

A simple scheme for the optimization of springs integrated into peristaltic mechanism of volumetric pump is suggested. Firstly, the material properties of the tube involved in the mechanism are defined on the base of natural experiment and its finite element modelling. The formulated inverse identification problem is treated as an optimization problem. Secondly, for the particular peristaltic mechanism (the cam's shape plays the most important role here) by means of finite element modelling the necessary closure displacement and corresponding compression force is obtained.

To investigate the objective function landscape and to solve the optimization problem defined *Genetic algorithm* as a global optimization method was employed. Since the landscape of the objective function is exponentially decreasing without any local minima, the algorithm reached the target value after 9 generations by having population size of 20.

The resultant spring stiffness is obtained via simple engineering formula. The obtained resultant spring stiffness is optimal because the tube will not be under-compressed, since the resultant spring stiffness k appears at the closing point region. On the other hand, the tube will not be over-compressed, since the tube compression after the closing point region is absorbed by the springs.

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PVC MEDŽIAGOS SAVYBIŲ NUSTATYMAS SPRENDŽIANT STATINĮ ATVIRKŠTINĮ UŽDAVINĮ GENETINIŲ ALGORITMU

R e z i ū m ė

Projektuojant medicinos įrangą, būtina žinoti jos komponentų mechanines savybes. Tokia įranga, pvz., volumetrinis siurblys, naudoja peristaltinį mechanizmą, suspaudžiantį vadinamąjį IV agregatą, gaminamą iš PVC. Kadangi gamintojas PVC mechaninių savybių nenurodo, bandyta jas nustatyti sprendžiant atvirkštinį statinį uždavinį. Atvirkštinis uždavinys faktiškai yra optimizavimo uždavinys, kuriam spręsti parinktas genetinis algoritmas, kartu leidžiantis ištirti ir uždavinio tikslo funkcijos pavidalą. Be to, kartu apskaičiuotas ir optimalus peristaltinio mechanizmo spyruoklių standis.

R. Puiša, R. Belevičius

GRADING THE PVC MATERIAL BY SOLVING A STATIC INVERSE PROBLEM WITH GENETIC ALGORITHM

S u m m a r y

When developing hi-tech medical equipment the exact technical properties of its components must be known. Such an equipment as volumetric pump uses peristaltic mechanism compressing an intro-vein set, which is made from PVC material. Since needed mechanical properties of PVC material are not provided by its manufacturer, we aimed at finding them by solving an inverse static problem. The inverse problem appeared to be an optimization problem, therefore Genetic algorithm was chosen as an optimizer, which also let to investigate the problem landscape. In addition, a study of mechanical properties of PVC material helped to calculate optimal stiffness of the springs used in the mentioned peristaltic mechanism.

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ОПРЕДЕЛЕНИЕ СВОЙСТВ МАТЕРИАЛА ПВХ ПУТЕМ РЕШЕНИЯ ОБРАТНОЙ СТАТИЧЕСКОЙ ЗАДАЧИ ГЕНЕТИЧЕСКИМ АЛГОРИТМОМ

Р е з ю м е

При проектировании медицинского оборудования необходимы механические свойства ее компонентов. Такое оборудование, как волнометрическая помпа, использует перистальтический механизм, сжимающий так называемый ИВ агрегат, изготовляемый из ПВХ. Изготовитель ПВХ не указывает механических свойств материала, поэтому они определены путем решения обратной статической задачи. Обратная задача фактически является задачей оптимизации, для чего подобран генетический алгоритм. Этот алгоритм наряду с решением задачи оптимизации также позволяет исследовать вид функции цели. Рассчитана оптимальная жесткость пружин перистальтического механизма.

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