

EVOLUTIONARY IDENTIFICATION OF MICROSTRUCTURE PARAMETERS IN THE THERMOELASTIC POROUS MATERIAL

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The work is devoted to the identification of microstructure parameters of a porous body under thermal and mechanical loads. The goal of the identification is to determine the parameters of the microstructure on the basis of measurements of displacements and temperatures at the macro level. A two-scale 3D coupled thermomechanical model of porous aluminum is considered. The representative volume element (RVE) concept modeled with periodical boundary conditions is assumed. Boundary-value problems for RVEs (micro-scale) are solved by means of the finite element method (FEM). An evolutionary algorithm (EA) is used for the identification as the optimization technique.

Keywords: thermoelasticity, identification, numerical homogenization, evolutionary algorithms

1. Introduction

Multiscale modeling is a vital technique in the process of designing new, advanced materials, where desired material properties or geometric configurations of the microstructure are sought. Thanks to multiscale modeling, it is possible to simulate behavior of these materials utilizing suitable methods for scales of different magnitudes. Trying to simulate details of geometry of some structures in one scale can result in a very complex model. In such a case, numerical simulations are very time consuming or even impossible, so multiscale modeling can be applied to reduce the complexity of the model concerning two or more scales. Many effects can be considered in the multiscale model: in the macro level, mechanical and thermal loads, in the meso- and micro-scale, phase inclusions or porosity and even defects in the crystal lattice. It is possible to achieve coupling between numerical simulations and molecular dynamics as well (Auriault *et al.*, 2009; Fish, 2006, 2008). To simulate the behavior of a material in lower scale, it is necessary to transfer the information on quantities such as strains or temperatures from a higher to the lower scale. The information on efficient material parameters are determined experimentally, analytically or by means of numerical homogenization methods in the microscale and transferred to the macroscale. Experimental methods require manufacturing a real model of a considered structure and complicated measurements of sought quantities. An analytical method can be applied only to simple models. Numerical homogenization (Buyrachenko, 2007; Fish, 2006; Zhodi and Wriggers, 2008) using the boundary element method (BEM) (Ptaszny and Hatlas, 2018) or the finite element method (FEM) (Qiang *et al.*, 2018) on the other hand is a very efficient and popular method. The identification problem may deal with searching of desired material properties, shape or position of inclusions or voids in the structure. In the case of considering a multiphysics problem, material properties related to multiple fields (e.g. mechanical, thermal) are sought (El Moumen *et al.*, 2015; Zhuang *et al.*, 2015, Živcová *et al.*, 2009). Identification functionals have to be defined to solve an identification problem. If these functionals are solved numerically, they are often strongly multi-modal, in particular for coupled

problems. To solve the identification problem, an efficient optimization technique able to deal with multi-modal problems is necessary. One of approaches capable of dealing with such problems are evolutionary algorithms (EAs) (Ogierman and Kokot, 2016). A significant benefit of using this method is its ability to find solutions both near local optima and in the entire space of admissible solutions.

In this paper, a problem of identification of parameters of numerically homogenized microstructure for porous materials by means of an evolutionary algorithm is presented. Identification functionals are numerically determined by means of FEM. Input data for the identification problem is based on information on thermal and mechanical fields measured by temperature and displacement sensors on the boundary of the examined structure in the macro level. This work is an extension of the previous works in which identification and optimization tasks have been solved for 2D and 3D structures with cylindrical inclusions (Długosz, 2014; Długosz and Burczyński, 2013; Długosz and Schlieter, 2013).

2. Formulation of the problem

The purpose of identification is to determine parameters of the microstructure on the basis of measurements carried out in a macroscale. The model of a two-scale porous material with global periodicity is considered (Kouznetsova *et al.*, 2004; Terada *et al.*, 2010).

In the problem of identification, a set of parameters of the microstructure is sought on the basis of quantities measured in the macroscale. The two-scale porous material model with global periodicity is considered (Fig. 1).

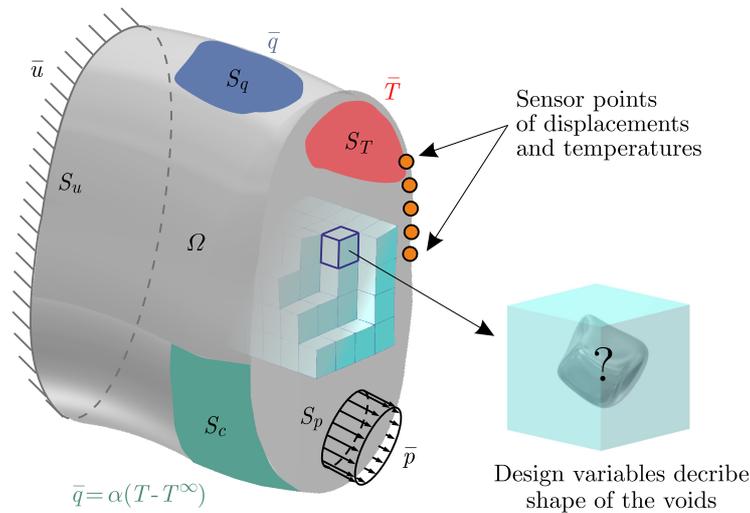


Fig. 1. A two-scale model of a thermoelastic porous body with imposed thermomechanical boundary conditions

It is assumed that there is a known set of experimentally measured values in selected points on the boundary of a considered object and a corresponding set of values obtained by means of numerical homogenization. The values of displacement and temperature are measured at points where sensors are located on the real object. Authors highlight the fact that no real experiment was carried out and both experimental and theoretical values are determined using a numerical simulation. To overcome this difficulty, changes in the location of sensors or an increased number or measurement of quantities coming from different physical fields are proposed. It was reported that in the case of identification problems measuring values related to both mechanical and thermal fields is advantageous compared to measuring only temperatures or only displacements (Burczyński *et al.*, 2006).

In the identification task, the aim was to find the shape of the void in the microstructure on the basis of temperature and displacement measured in the macro-scale (Fig. 1). The identification functional was defined as

$$I_0 = a \sum_{i=1}^m (\hat{u}_i - u_i)^2 + b \sum_{j=1}^s (\hat{T}_j - T_j)^2 \quad (2.1)$$

where m is the number of displacement sensor points, s – number of temperature sensor points, \hat{u} and \hat{T} are known values of displacement and temperature in the sensor points, u and T are displacement and temperature values in the sensors obtained on the basis of numerical simulation, a and b are weight coefficients assuring a comparable share of displacement and temperature parts in the identification problem.

Numerical homogenization using RVE concept and FEM is carried out in order to solve the two-scale thermoelastic problem for a porous structure. The purpose of homogenization is to find effective material properties of a non-homogenous structure and thus establish the relationship between macroscopic quantities. In the case of thermo-elastic problems, the determined properties can be for example elasticity constants, thermal expansion coefficients or thermal conductivity coefficients (Terada *et al.*, 2010). The thermal expansion coefficient is constant regardless of a geometric configuration of the porous microstructure, so it is redundant to homogenize it. In this paper, a linear thermoelasticity problem described by partial differential equations of heat conduction and elasticity, considering thermal strains is examined (Beer, 1983; Carter and Booker, 1989; Nowacki, 1972; Zienkiewicz and Taylor, 2005)

$$kT_{,ii} = 0 \quad \mu u_{i,jj} + (\mu + \lambda)u_{j,ji} - (3\lambda + 2\mu)\alpha_T T_{,i} = 0 \quad (2.2)$$

where k is thermal conductivity, T is temperature, u is displacement, α_T is linear expansion coefficient, μ and λ are Lamé constants.

Equations (2.2) have to be supplemented by mechanical boundary conditions

$$\Gamma_t : t_i = \bar{t}_i \quad \Gamma_u : u_i = \bar{u}_i \quad (2.3)$$

and thermal boundary conditions

$$\Gamma_T : T_i = \bar{T}_i \quad \Gamma_q : q_i = \bar{q}_i \quad \Gamma_c : q_i = \alpha(T_i - T^\infty) \quad (2.4)$$

where \bar{u}_i , \bar{t}_i , \bar{T}_i , \bar{q}_i , α , T^∞ are known: displacements, tractions, temperatures, heat fluxes, heat conduction coefficient and ambient temperature, respectively.

An example of boundary conditions which can be imposed on the model are shown in Fig. 1. Equations (2.2) supplemented by boundary conditions are solved by means of FEM in a discrete space and are transformed to a set of algebraic equations in the matrix form

$$\mathbf{K}_T \mathbf{T} = \mathbf{Q} \quad \mathbf{K}_M \mathbf{U} = \mathbf{F} + \mathbf{F}_T \quad (2.5)$$

where \mathbf{K}_T is the global thermal conductivity matrix, \mathbf{K}_M is the global stiffness matrix, \mathbf{T} , \mathbf{Q} , \mathbf{U} and \mathbf{F} are nodal vectors of temperatures, heat fluxes, displacements and applied forces respectively. \mathbf{F}_T is the nodal vector of forces due to the thermal strain vector.

Following the assumptions taken into consideration in the process of numerical homogenization using RVE:

— principle of scale separation

$$\frac{l}{L} \ll 1 \quad (2.6)$$

where l and L are characteristic dimensions of a structure in a micro- (RVE) and macroscale,

— the averaging of quantities is carried out according to the averaging theorem

$$\langle \cdot \rangle = \frac{1}{|\Omega_{RVE}|} \int_{\Omega_{RVE}} (\cdot) d\Omega_{RVE} \quad (2.7)$$

where $\langle \cdot \rangle$ denotes the average macroscopic value of a given field over the volume V of the RVE,
 — Hill's condition: the equality of the averaged micro-scale energy density and the macro-scale energy density at the selected point of macro-structure corresponding to the RVE

$$\langle \boldsymbol{\sigma}_{ij} \boldsymbol{\varepsilon}_{ij} \rangle = \langle \boldsymbol{\sigma}_{ij} \rangle \langle \boldsymbol{\varepsilon}_{ij} \rangle \quad (2.8)$$

where $\boldsymbol{\sigma}_{ij}$, $\boldsymbol{\varepsilon}_{ij}$ are stress and strain tensors, respectively.

For the heat conduction problem, the Hill condition takes the form

$$\langle \mathbf{T}_{,i} \mathbf{q}_i \rangle = \langle \mathbf{T}_{,i} \rangle \langle \mathbf{q}_i \rangle \quad (2.9)$$

where $\mathbf{T}_{,i}$ and \mathbf{q}_i are temperature gradient and heat flux, respectively.

Numerical homogenization by FEM is used in the microscale. Periodic boundary conditions are imposed on the RVE. Average stresses and heat fluxes obtained from FEM analysis of RVE are used to determine the effective material properties according to equation (2.7). Hooke's law in the microscale takes the following form

$$\langle \boldsymbol{\sigma}_{ij} \rangle = \mathbf{c}'_{ijkl} \langle \boldsymbol{\varepsilon}_{ij} \rangle \quad (2.10)$$

and Fourier's law in the microscale

$$\langle \mathbf{q}_i \rangle = \mathbf{k}'_{ij} \langle \mathbf{T}_{,i} \rangle \quad (2.11)$$

The tensor of elastic constants \mathbf{c}'_{ijkl} (using Voight notation) of the RVE is described by a set of nine independent constants and takes the following form

$$\mathbf{c}'_{ij} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{21} & c_{22} & c_{23} & 0 & 0 & 0 \\ c_{31} & c_{32} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} \quad (2.12)$$

whereas the tensor of thermal conductivity coefficients \mathbf{k}'_{ij} for non-crystalline anisotropic materials is described by 3 independent constants and takes the form

$$\mathbf{k}'_{ij} = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix} \quad (2.13)$$

It is necessary to perform six analyses to determine the effective elastic constants and three analyses to determine the effective thermal constants. Each column or row of the tensor of effective elastic constants is obtained by applying the initial unitary strain to the RVE model and for the tensor of effective thermal constants likewise. MSC.Mentat/Marc software was used to perform FEM computations in both scales and in-house procedures implemented in C++ programming language and internal MSC script language were used to enhance the automatic generation of models for the multiscale analyses (MSC.MARC, 2017).

To verify the accuracy of the proposed method, the numerical homogenization results were compared to other methods of determining effective elastic and thermal properties. The RVE

model of a 3D cube with a spherical void was considered. Such a structure can be described with isotropic thermal and mechanical properties. The model made of aluminum with voids filled with air is considered. Thermal conductivity of air is multiple magnitudes lower than of aluminum and thus is neglected. Furthermore, the effects of radiation and convection are also neglected as they play a minor role compared to the heat conduction in aluminum. The obtained values of effective Young's modulus and effective thermal conductivity are compared to the results obtained using rule of mixtures, Hashin-Strikman and Mori-Tanaka model. The relation between effective material properties to the porosity of the model for these methods is shown in Figs. 2 and 3. The results are satisfactory, and the developed method can be considered positively verified.

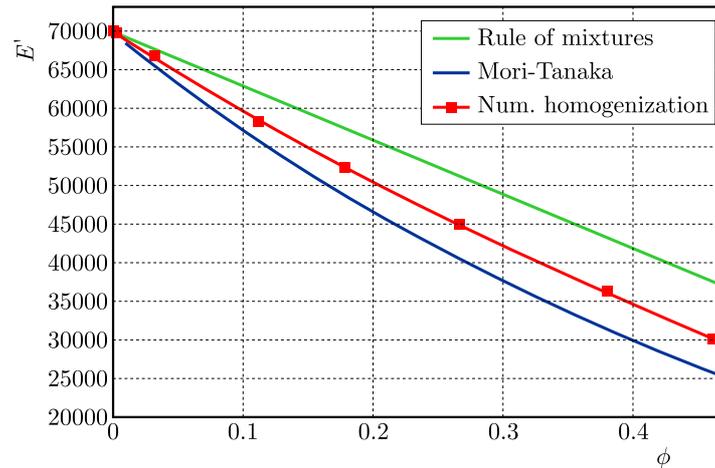


Fig. 2. Relations between Young's modulus and the porosity

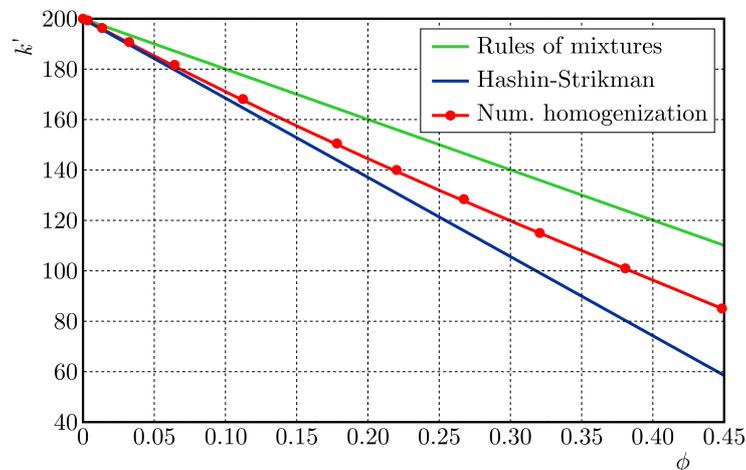


Fig. 3. Relations between the thermal conductivity and the porosity

3. Identification algorithm

The determination of the parameters of the microstructure is based on minimizing the norm between measured and computed values of temperature (2.1). The minimization procedure is performed by means of an evolutionary algorithm (genetic algorithm with real-coded value of genes, not binary strings, are used). Application of EAs (one of the most popular global optimization techniques) has several advantages compared to classical optimization techniques. For example, a fitness function does not have to be continuous, information about the objective function gradient is not necessary, the choice of the starting point may not influence the convergence

of the method, and regularization methods are not needed (Michalewicz, 1992; Michalewicz and Fogel, 2004). An in-house implementation of EA was used. The solutions of the problem are specified by the chromosomes in EA. Chromosome genes represent design parameters responsible for the shape of the void in the microstructure or values of material parameters. The following evolutionary operators were implemented: uniform, boundary and Gaussian mutation, simple and arithmetic crossover, and the rank selection method. Implementation of the Gaussian mutation significantly decreases the risk of sticking the algorithm in a local minimum (Carter and Booker, 1989). This algorithm was tested on several mathematical benchmark problems and real engineering problems as well, obtaining satisfactory results.

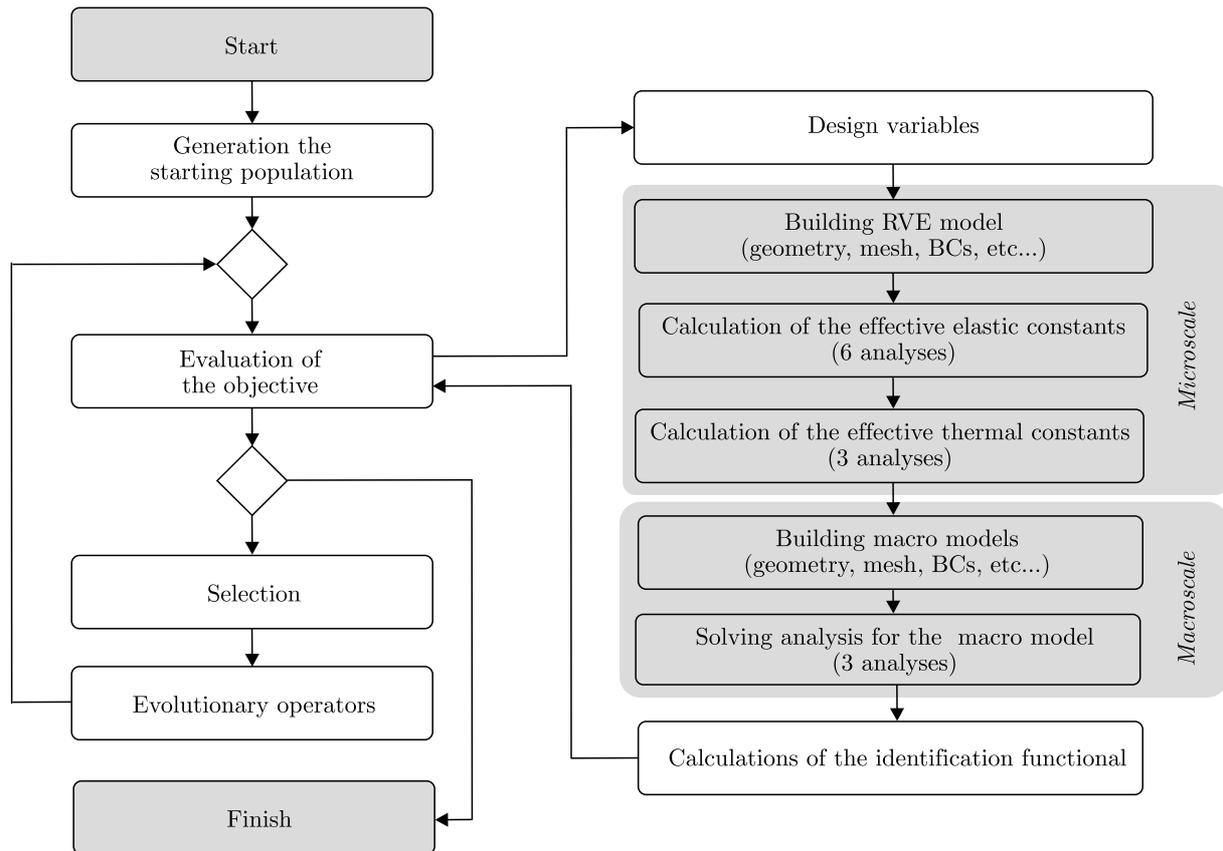


Fig. 4. Flow chart of the developed evolutionary identification procedure

The evolutionary algorithm starts with a population of chromosomes randomly generated. For each individual, an objective function (identification functional I_0) is determined. On the basis of chromosomes genes, which are design variables responsible for the shape of the void in the microstructure, an RVE model is created. A detailed description of the generation internal structure of the RVE is given in the next Section. Creation of the RVE is aided by procedures written for preprocessor Mentat. Next, calculation of the components of tensor of elastic constants (2.12) and heat conduction coefficients (2.13) is performed. This requires a total of nine tasks to be solved for the microstructure model. Next, the calculated components of the elastic and thermal conductivity tensors are used for building the macro model. For the numerical example of identification included in the present paper, three thermoelastic analyses of the macrostructure are solved. On the basis of the obtained results for such analyses, the functional I_0 (2.1) is calculated. The algorithm works until the stop condition is not fulfilled (maximal number of generations is assumed in the paper). Figure 4 shows flow chart of the entire evolutionary identification procedure.

4. Numerical example

4.1. Macromodel

A cube of dimension $20 \times 20 \times 20$ mm is modeled as a macromodel. The model is thermomechanically loaded along all normal directions. For each direction, nodes belonging to one surface are fixed in all degrees of freedom (u_0), while the opposite surface is loaded with pressure $p_0 = 100$ MPa. In the case of thermal boundary conditions, on the fixed surface a constant temperature $T_0 = 100^\circ\text{C}$ is applied, whereas on the opposite side heat flux $q_0 = -100$ mW/mm² is applied (Fig. 5). Sensor points of displacement and temperatures are located on the edges of the cube parallel to the loading direction. For each load case six sensors are applied to the particular edge, which gives the total number of sensor equal to 72. Three separate boundary-value problems of thermoelasticity are solved for each calculation of the identification functional.

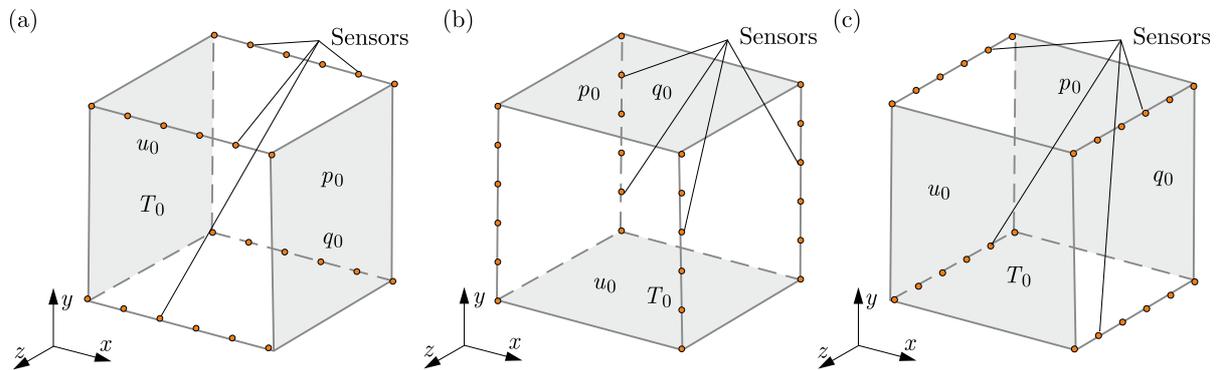


Fig. 5. Macromodel of the cube thermomechanically loaded along: (a) x axis, (b) y axis, (c) z axis

4.2. Micromodel of the RVE

The micromodel is a cube with the periodic boundary conditions. The void inside the RVE is modelled by means of a B-spline. The void can be rotated in two perpendicular planes. It allows one to obtain the shape of the void with almost an arbitrary shape. The first step of creation of the void is generation of the curve of length L , next on the basis of three control points a parametric B-spline curve is created. Next, the surface created between these curves is revolved, obtaining the shape of the void, which can be additionally rotated in the two perpendicular planes. The consecutive stages of the creation of the void are presented in Fig. 6. It can be seen that the void is parametrized by means of six design variables. The RVE size used in the micro-model is 1 mm, whereas the size and shape of the void is generated taking into account box constraints imposed on design variables (Table 1).

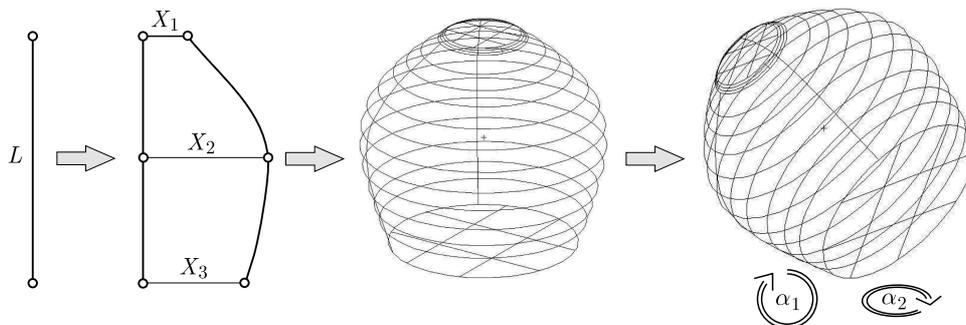


Fig. 6. Stages of the creation of the void in the micromodel

Table 1. Box constraints imposed on design variables

	L [mm]	x_1 [mm]	x_2 [mm]	x_3 [mm]	a_1 [°]	a_2 [°]
min	0.1	0.05	0.05	0.05	0	0
max	0.6	0.35	0.35	0.35	90	90

4.3. Variants of the identification task

Nine variants for different shapes and orientations of the void have been performed. Various shapes of the void for each case can allow one to test the efficiency of the identification procedure. For all variants, the evolutionary algorithm was run with the following parameters: population size 10; number of iterations 100; probability of simple crossover 0.1; probability of arithmetic crossover 0.1; probability of uniform mutation 0.1; probability of Gaussian mutation 0.7; rank selection pressure coefficient 0.8. Table 2 contains comparison between values of the design variables found by the proposed method with comparison to the exact solution. Figures 7 and 8 graphically presents the results of the identification for all nine variants.

Table 2. Exact and identified design variable values for all identification variants

		L [mm]	x_1 [mm]	x_2 [mm]	x_3 [mm]	a_1 [°]	a_2 [°]
Variant 1	Exact	0.6	0.35	0.35	0.35	0	0
	Found	0.6	0.35	0.35	0.35	0	0
Variant 2	Exact	0.6	0.35	0.35	0.35	45	45
	Found	0.6	0.35	0.35	0.35	44.51	45.23
Variant 3	Exact	0.1	0.05	0.05	0.05	45	45
	Found	0.1	0.05	0.05	0.05	44.9	43.37
Variant 4	Exact	0.1	0.05	0.35	0.05	0	0
	Found	0.11	0.29	0.16	0.057	2.03	3.34
Variant 5	Exact	0.1	0.05	0.35	0.05	90	0
	Found	0.1	0.079	0.20	0.29	90	24.49
Variant 6	Exact	0.4	0.1	0.2	0.3	0	90
	Found	0.38	0.28	0.11	0.26	12.21	72.63
Variant 7	Exact	0.5	0.3	0.3	0.3	30	60
	Found	0.54	0.31	0.32	0.21	30.5	61.11
Variant 8	Exact	0.3	0.3	0.1	0.1	20	80
	Found	0.16	0.31	0.17	0.2	22.25	73.46
Variant 9	Exact	0.4	0.2	0.2	0.2	45	45
	Found	0.47	0.11	0.21	0.2	40.18	40.29

For variants 1, 2 and 3 the accuracy of identification is very high. Analyzing the results, collected in Table 2, only the first three variants can be treated as satisfactory, but even for the variants where particular design variables have not been perfectly identified (variants 4, 5, 7 and 9), the results show similarity of the shape (see Figs. 7 and 8) and could be treated as acceptable. It has to be underlined that for some cases, the accuracy of identification is not satisfactory (variants 6 and 8).

5. Conclusions and final remarks

A method of identification of parameters of a microstructure on the basis of measurements at the macro level for porous materials under thermomechanical load has been presented. Procedures

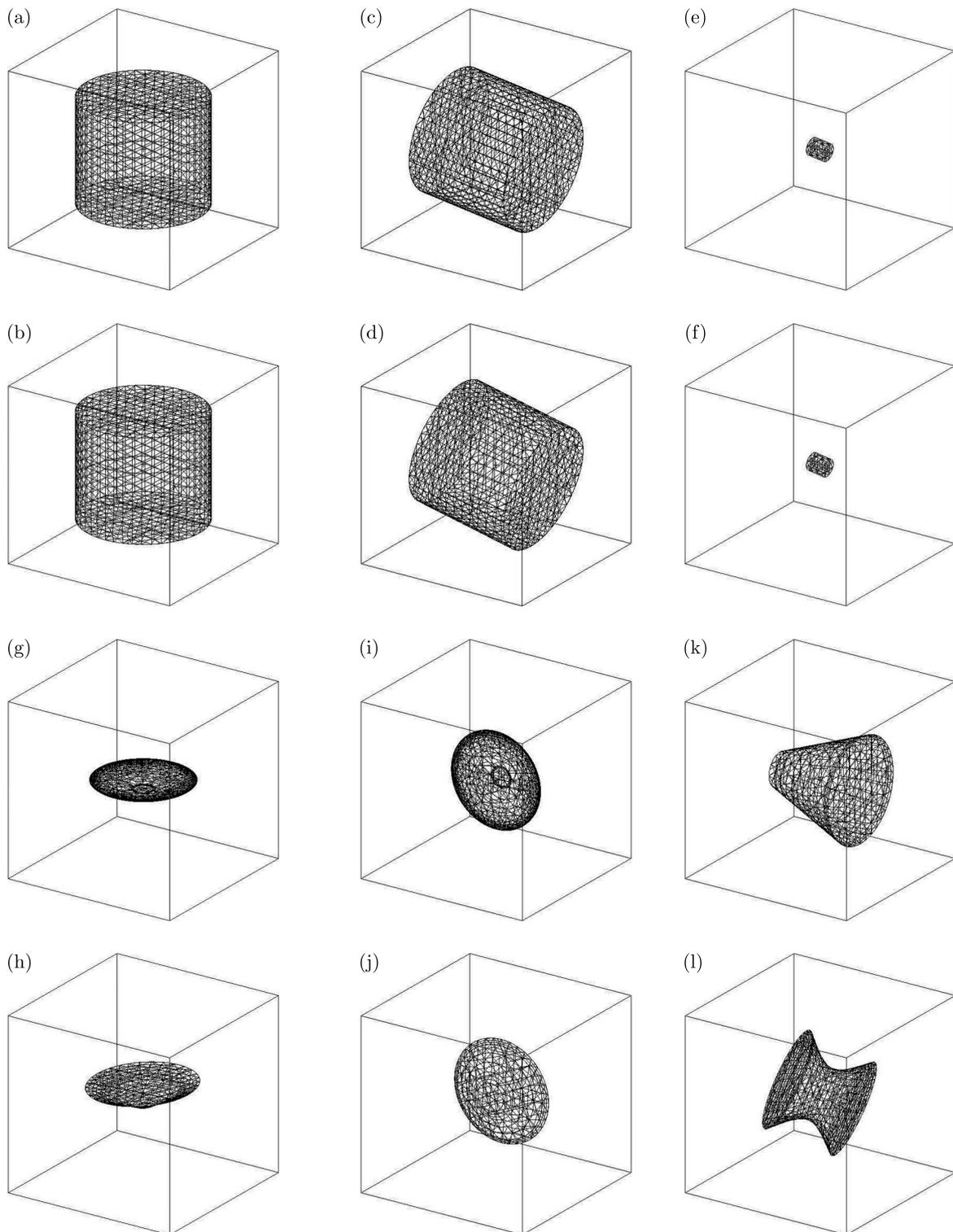


Fig. 7. Shape of the microstructure for performed variants of identification: (a) variant 1 – exact, (b) variant 1 – found, (c) variant 2 – exact, (d) variant 2 – found, (e) variant 3 – exact, (f) variant 3 – found, (g) variant 4 – exact, (h) variant 4 – found, (i) variant 5 – exact, (j) variant 5 – found, (k) variant 6 – exact, (l) variant 6 – found

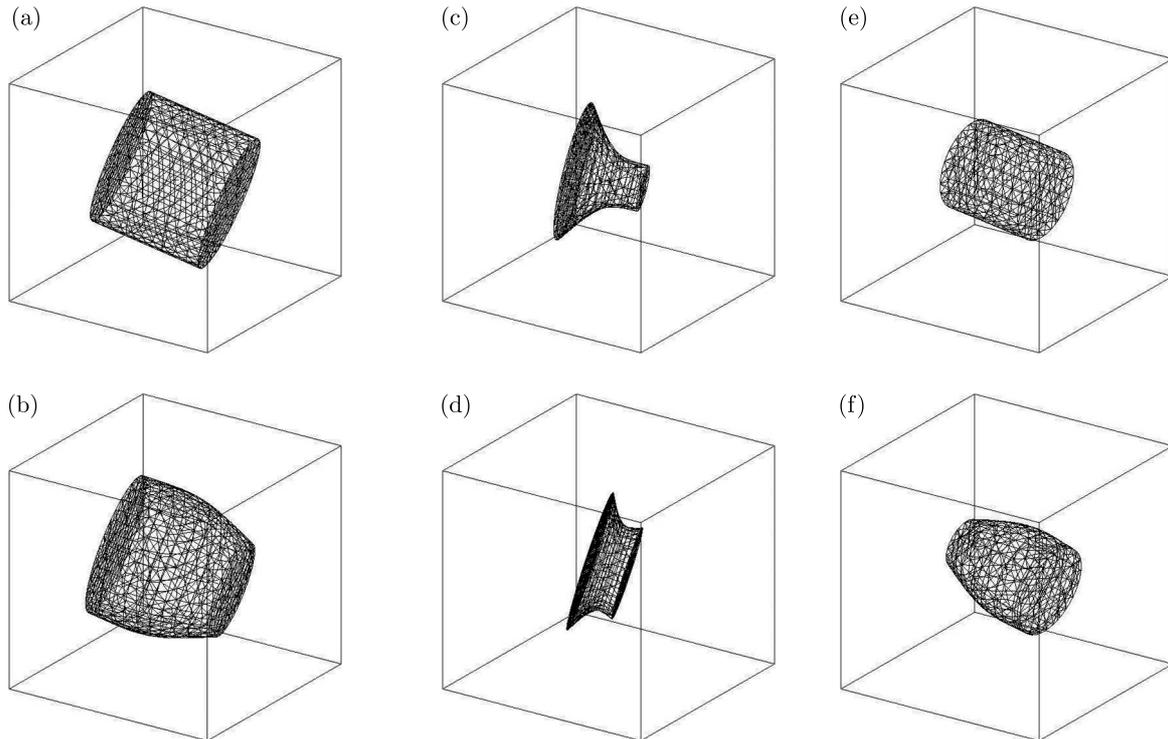


Fig. 8. Shape of the microstructure for performed variants of identification: (a) variant 7 – exact, (b) variant 7 – found, (c) variant 8 – exact, (d) variant 8 – found, (e) variant 9 – exact, (f) variant 9 – found

for numerical homogenization with the RVE concept and FEM have been successfully verified and used in identification tasks. Parametrization of the void in the microstructure, aided by parametric curves (B-splines), allows one to generate a void with a shape that can be changed very flexibly. The identification functional which depends on measurements of temperatures and displacements in boundary sensor points was proposed and implemented. For solving the identification tasks, the system which combines in-house implementation of evolutionary algorithms and developed procedures for the calculation of the identification functional has been built. Nine variants of identification tasks for different shapes and orientations of the void in the microstructure have been performed. The presented method of identification gives very good or acceptable results for majority of the considered identification variants. The proposed method of parametrization allows one to create a similar shape of the voids for different values of particular design variables. It can be concluded that by increasing the flexibility of generation of the shape of the voids (which is one of the goals of this paper), ambiguity of the identification increases as well. Evolutionary algorithms belong to the group of methods which are not affected by getting stuck in local minima, but when the response of the system in thermal and mechanical parts is very seminal for different shapes of the void, it can lead to ambiguity in the solution. In order to reduce this negative aspect, more information from the measurements should be introduced. In the present paper, instead of typically solved single boundary-value problem, the multiloading (3 load cases) is proposed. Comparing to the case when the functional is calculated on the basis of the single boundary-value problem (Długosz and Burczyński, 2013), the proposed multiloading approach gives significantly better results. Detailed comparison between such an approach for 3D models is not included in the paper. Despite obtaining acceptable satisfactory results of the identification for majority of the cases, the proposed method should be improved. The future tasks will be related to checking of the proposed identification methods for noisy data measured in sensors of temperatures and displacements, the application of more sophisticated thermal and

mechanical load cases for the micromodel, and checking of the influence of changing locations and the number of sensors.

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