COMPUTER METHODS IN MATERIALS SCIENCE

2022, vol. 22, no. 3, 107–114
https://doi.org/10.7494/cmms.2022.3.0784

Multiobjective optimiaztion of microstructure parameters in a thermoelastic porous material by means of differential evolution and elements of game theory

Adam Długosz*, Tomasz Schlieter

Silesian University of Technology, Department of Computational Mechanics and Engineering, Gliwice, Poland.

Abstract

The paper is devoted to the optimization of the microstructure parameters of a porous medium under thermo-mechanical loading. Four different criteria related to the properties of the porous material have been proposed and numerically implemented. To solve a multiobjective problem, a novel method based on the coupling of differential evolution and elements of game theory is used. The proposed algorithm features an appropriate balance between exploration and exploitation of objective space, which is necessary for the successful optimization of these types of tasks with the use of numerical simulations. The model of the thermo-elastic porous material is composed of two-scale direct analysis based on a numerical homogenization. Direct thermoelastic analysis with representative volume element (RVE) and finite element method (FEM) is performed. Numerical example of the optimization illustrating the usefulness of the proposed method is included.

Keywords: multiobjective optimization, thermoelasticity, porous materials, multiscale problem, representative volume element, differential evolution, game theory

1. Introduction

A multiscale analysis is an important method in the design process of advanced materials, one in which geometry and properties of microstructure are taken into consideration. The microstructure of materials can strongly influence physical properties, such as strength, heat conductivity, electrical conductivity, density etc. Microscale characteristics play a crucial role in the behavior of materials such as porous materials or materials reinforced with fibers or particles. A microstructure composed of more than one material with dissimilar physical properties can provide properties which would not be available to be obtained using a homogenous material (Buryachenko, 2007; Zohdi & Wriggers, 2005). The numerical simulation of such structures in one scale is a very computationally demanding task as it would require extremely fine mesh and complex models in order to adequately reflect the differences in properties of the microstructure sections. For this reason, multiscale modelling can be applied to reduce the complexity of models concerning two or more scales. Many phenomena happening on a different magnitudes of scale and interacting with each other can be investigated in the multiscale model. For example, on the macroscale, we can investigate mechanical and thermal boundary conditions (loads, supports etc.), whie in the meso- and microscales, we

* Corresponding author: adam.dlugosz@polsl.pl
ORCID ID's: 0000-0003-4529-4201 (A. Długosz), 0000-0001-9855-050X (T. Schlieter)

can identify inclusions, cavities and even defects in the crystal lattice (Auriault et al., 2009; Fish, 2006). Multiscale modelling can even be used in problems concerning effects at a molecular level. In order to analyze the behavior of a system at the macroscale it is necessary to establish information on effective material properties. In the process of homogenization, a heterogenous material is transformed into a homogenous one described by effective material properties obtained through microscale analyses. In the case of a simple microstructure geometry, analytical solutions can be used, although it is necessary to employ numerical methods for more complex shapes. The boundary element method was used to perform numerical homogenization of porous structures (Ptaszny & Hatłas, 2018), however, FEM is the most popular method used for numerical homogenization due to its universal applicability and availability in the CAE software. Multiobjective optimization problems concerning multiscale models are remarkably demanding computational tasks. During the optimization process, in order to search the solution space for desirable designs, it is necessary to obtain values of optimization functions multiple times. In the case of a multiscale problem, each analyzed candidate solution additionally requires multiple analyses at the microscale to perform numerical homogenization. For this reason, an efficient multiobjective optimization tool is crucial to govern the optimization process in such a problem to achieve satisfying results in a limited time. This paper is an extension of the previous works in this area, in which different optimization methods and models of porous media were considered (Długosz, 2014; Długosz & Schlieter, 2016, 2018).

2. Formulation of the two-scale thermo-elastic problem

Numerical homogenization utilizing the RVE concept and FEM is carried out to solve the two-scale thermo-elastic problem for a porous structure. The aim of homogenization is to determine effective material properties of a non-homogenous structure and use them to solve macroscale problems. For thermo-elastic problems, the determined properties include elasticity constants, thermal expansion coefficients or thermal conductivity coefficients. The thermal expansion coefficient does not require homogenization in analyzed example, as it does not depend on the geometric configuration of the microstructure (Terada et al., 2010). The linear thermoelasticity problem is described by a set of partial differential equations of heat conduction and elasticity, considering thermal strains (Beer, 1983):

$$kT_{,ii} = 0 \tag{1}$$

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

where: k – thermal conductivity; T – temperature, u – displacement; α_T – linear expansion coefficient; μ, λ – Lamé constants.

The boundary of the body is defined by the parts of the boundary where thermal and mechanical boundary conditions are applied. To solve the thermo-mechanical boundary value problem, FEM is used (Zienkiewicz et al., 2005). Partial differential equations governing the problem are discretized and transformed into a system of algebraic equations. After taking into consideration boundary conditions, a resulting system of equations in the matrix form is obtained:

$$\mathbf{K_T T} = \mathbf{Q} \tag{3}$$

$$\mathbf{K_M U} = \mathbf{F} + \mathbf{F_T} \tag{4}$$

where: $\mathbf{K_T}$, $\mathbf{K_M}$ – global matrices of thermal conductivity and stiffness, respectively, assembled by the aggregation of local matrices according to the FEM discretization scheme; $\mathbf{T}$, $\mathbf{Q}$, $\mathbf{U}$, $\mathbf{F}$ – global vectors of temperatures, heat fluxes, displacement, and mechanical loads, respectively; $\mathbf{F_T}$ – a vector of loads due to thermal strain obtained on the basis of a temperature gradient from Equation (3).

As weak coupling between physical fields is assumed, thermal and mechanical analyses are solved in a successive manner. Coupling is realized by transferring loads into subsequent analyses. A set of assumptions is taken into consideration in the process of numerical homogenization using RVE, including:

– principle of scale separation:

$$\frac{l}{L} << 1 \tag{5}$$

where l and L are characteristic dimensions of the RVE and in the macro scale;

– averaging theorem:

$$\langle \cdot \rangle = \frac{1}{|\Omega_{RVE}|} \int_{\Omega_{RVE}} (\cdot)\, d\Omega_{RVE} \tag{6}$$

where $\langle \cdot \rangle$ denotes the average of a given field over the volume V of the RVE;

– Hill condition provides 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:

$$\langle \sigma_{ij} \varepsilon_{ij} \rangle = \langle \sigma_{ij} \rangle \langle \varepsilon_{ij} \rangle \tag{7}$$

where σ_{ij} and ε_{ij} are stress and strain tensors, respectively.

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

$$\langle T_{,i} \, q_i \rangle = \langle T_{,i} \rangle \langle q_i \rangle \tag{8}$$

where $T_{,i}$ and q_i are temperature gradient and heat flux, respectively.

Numerical homogenization using the RVE approach with periodic boundary conditions is used. FEM analysis in the microscale is performed to obtain average stress and heat fluxes in RVE to determine the effective material properties according to Equation (6).

Hooke's law in the microscale takes the following form:

$$\langle \sigma_{ij} \rangle = c'_{ijkl} \langle \varepsilon_{ij} \rangle \tag{9}$$

$$\langle q_i \rangle = k'_{ij} \langle T_{,i} \rangle \tag{10}$$

The tensor of elastic constants c'_{ijkl} is symmetric. The RVE is described by 9 independent material constants for 3D problems. Using Voight notation, the tensor of elastic constants can be written in the form:

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

The tensor of heat conduction coefficients k'_{ij} for non-crystalline anisotropic materials takes the form:

$$k'_{ij} = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix} \tag{12}$$

Determining effective elastic constants requires running six analyses for the elasticity problem and the determination of effective thermal constants and three analyses of the heat conduction problem. Initial unitary strain is applied to the RVE model, and microscale analysis is performed to solve a single column or row of the tensor of effective elastic constraints. The same approach is used to calculate the values of elements of the tensor of effective thermal constants. In total, there are 9 microscale analyses required as a prerequisite to eventually solving a macroscale analysis resulting in obtaining a value of optimization functional. MSC Mentat/Marc software was used for FEM computations in both micro- and macroscale (MSC Software Corporation, 2019). Automatic generation of models for the multiscale analysis was performed utilising an in-house procedure implemented in the C++ programming language and internal MSC script language.

3. Optimization method

The idea of multiobjective optimization is not to optimize a single criterion, but a vector of criteria at the same time, thus a result of such an algorithm run is a set of non-dominated solutions obtained for the contradictory criteria. These solutions are optimal in the Pareto sense (Coello Coello, 2005). When designing the microstructure of a porous medium under thermal and mechanical loading, more than one criterion should obviously be considered. In the considered problem, four different criteria are proposed and formulated in the next paragraph. Such criteria calculated on the basis of numerical FEM calculations caused that functions are very often difficult to optimize using traditional optimization techniques. The main reasons for this are: contradiction between criteria, discontinuous objective space, non-convex of the Pareto fronts, existence of a large number Pareto fronts. Of course, the criteria defined in this way do not always have to have all the above-mentioned features, however, knowledge of their exact characteristics for real problems is difficult or impossible to be achieved. In such situations, a very good choice is to use methods based on metaheuristic algorithms (Vesterstrom & Thomsen, 2004). Moreover, metaheuristic algorithms (e.g. evolutionary methods) naturally process sets of solutions, so they are convenient to be used for multiobjective optimization tasks. A multiobjective optimization method which couples a differential evolution algorithm (Das & Suganthan, 2011; Storn & Price, 1997) and elements of game theory called DEGT is developed to solve considered a multiscale problem.

The idea behind coupling differential evolution and elements of a game theory comes down to treating objectives as players, playing a cooperative game, trying to improve their respective objectives with the resources given and sharing the information with each other, iteratively looking for a Nash equilibrium

(Fudenberg & Tirole, 1991; Osborne & Rubinstein, 1994). Each player is given a part of the design variable vector at random as their resource, while the rest of the vector is fixed and determined by other players' choices. To ensure the diversification of solutions, the assignment of resources is changed in a way that each design variable is modified by one and only one player. The assignment of resources is changed after each of the players makes his move. The player's move is to run the single-objective optimization process, using a differential evolution algorithm to improve one objective at a time using the resources allocated.

The general idea of DEGT is shown as a pseudocode in Figure 1. In the first step, a problem needs to be defined, including the expression of objective functions and design parameters. Players in the game are linked to certain objectives at this point. The first solution is sought concerning the first objective, and then the process is followed by playing consecutive cooperative games using the DE optimizer by each of the players. Optimization proceeds iteratively, new solutions are saved if they are non-dominated and otherwise discarded. After finishing satisfying the termination condition, the process is concluded with post-optimization tasks. The algorithm is comprehensively tested using typical benchmark functions and performance metrics and compared with the algorithms NSGA-II and NSGA-III. DEGT algorithm was proven to be efficient and competitive with the compared algorithms (Schlieter, 2021).

```
i ← 1
Perform single objective DE optimization on objective 1;
Save design variable vector of best solution S_i;
Calculate and save values of remaining objectives;
while termination condition
       if i% n_obj=1
                assign design variables to objectives;
       end-if
       Set values of fixed design variables according to solution S_i-1;
       Perform single objective DE optimization on objective 1+i% n_obj;
       Save design variable vector of best solution S_i;
       Calculate values of remaining objectives;
       if solution S_i is non-dominated
                save solution S_i;
                remove saved solutions dominated by S_i;
       end-if
       i ← i+1
end-while
```

Fig. 1. DEGT pseudocode

4. Formulation of the optimization criteria

Objectives in the optimization problem are devoted to the minimization of maximal displacements, minimization of maximal equivalent stress, maximization of the heat flux and maximization of porosity, which is related to the total mass and cost of the structure. These objectives are examples of conditions required of porous mechanical systems, although other criteria based on specific needs can be formulated. Values of functionals f_1 and f_2 used as objectives are computed using FEM simulations at macroscale, supplemented by FEM simulations at microscale, required in the process of numerical homogenization. Objectives f_3 and f_4 are obtained in the microscale. The geometry of the microstructure, described by design variables, is changed to fit the declared needs, formally described by Functionals (13)–(16):

– minimization of the maximal translational displacement of a system under a given load:

$$\min_x f_1 = \max(u) \tag{13}$$

– minimization of the maximal value of the equivalent (von Mises) stress of a system under a given load:

$$\min_x f_2 = \max(\sigma_{eq}) \tag{14}$$

– maximization of thermal conductivity in the direction along the axis of the bar:

$$\max_x f_3 = k_{11} \tag{15}$$

– maximization of porosity of the microstructure:

$$\max_x f_4 = \frac{\int_{\Omega_{por}} d\Omega_{por}}{\int_{\Omega_{RVE}} d\Omega_{RVE}} \tag{16}$$

Values of the aforementioned functionals are calculated numerically by means of FEM in MSC Patran/Nastran and MSC Marc/Mentat software based on a parametric model. Functionals f_1 and f_2 are calculated by running a static structural analysis under a given load. These functionals are obtained in macroscale analyses proceeded by a series of microscale analyses to establish values of effective material properties. Functional f_3 is calculated by running a thermal analysis of RVE at microscale. Functional f_4 is calculated on the basis of the geometry of the model at microscale and does not require solving any boundary-value problems. Problems of the maximization of f_3 and f_4 are transformed to minimization problems by multiplying a fitness function value by −1.

5. Numerical example

As an example of multi-criteria optimization of the microstructure of a porous material, the elementary geometry in the form of a cuboid solid at the macro scale was developed, while the void at the micro scale inside the RVE is modelled as a rotating solid using parametric curves. Cuboid aluminium solid of dimensions 100 mm × 20 mm × 20 mm is fixed on one side and subject to thermal and mechanical loads (Fig. 2). Uniform distributed load P is applied on the surface opposite of the fixed (displacement u_0) side. The temperature gradient for the model is realized by imposing on both these surfaces known temperatures T_1 and T_2. The boundary conditions and material properties of aluminium are presented in Table 1.

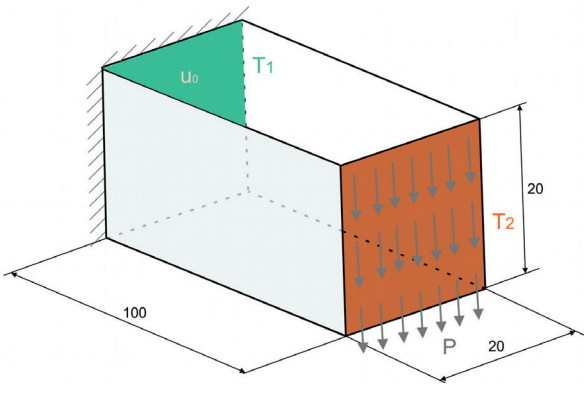

Fig. 2. Macromodel under thermal and mechanical loads

Table 1. Boundary conditions and material properties

Boundary condition or material property	Symbol	Value
Displacement	u_0	0
Load	P	360 N
Temperature 1	T_1	0°C
Temperature 2	T_2	100°C
Young's modulus	E	70 GPa
Poisson's ratio	ν	0.35
Thermal conductivity	K	200 W/(m·K)
Thermal expansion coefficient	α_t	$23 \cdot 10^{-6}$ K^{-1}

Analyses in the microscale concern the RVE model based on the parametric model in which the geometry of a microstructure is governed by a set of design variables, and are shown in Table 2 supplemented with limits imposed on them.

Table 2. Design variables

Symbol	Design variable	Lower limit	Upper limit
l	length of revolve axis	0.1	0.8
x_1	position of control point 1	0.01	0.3
x_2	position of control point 2	0.01	0.45
x_3	position of control point 3	0.01	0.45
x_4	position of control point 4	0.01	0.45
x_5	position of control point 5	0.01	0.3
α_1	rotation angle 1	0°	90°
α_2	rotation angle 2	0°	90°

The geometry of the RVE represents the geometry of a single pore in a periodic microstructure. A parametric model is developed in a way to provide a high flexibility of shapes, which can be described by a limited number of design variables. The geometry of the pore is assumed to be axisymmetric and is constructed by revolving a closed B-spline curve of order 4 around an axis. The shape of the curve is controlled by 5 design variables representing the position of control points (Fig. 3b), and the length of an axis is controlled by an additional design variable (Fig. 3a). After the pore volume is generated (Fig. 3c) it is furthermore rotated around two axes (Fig. 3d). The shape of a pore is eventually subtracted from the volume of a full unit block. After creating the geometry of an RVE, it is discretized using tet4 elements (Fig. 3e).

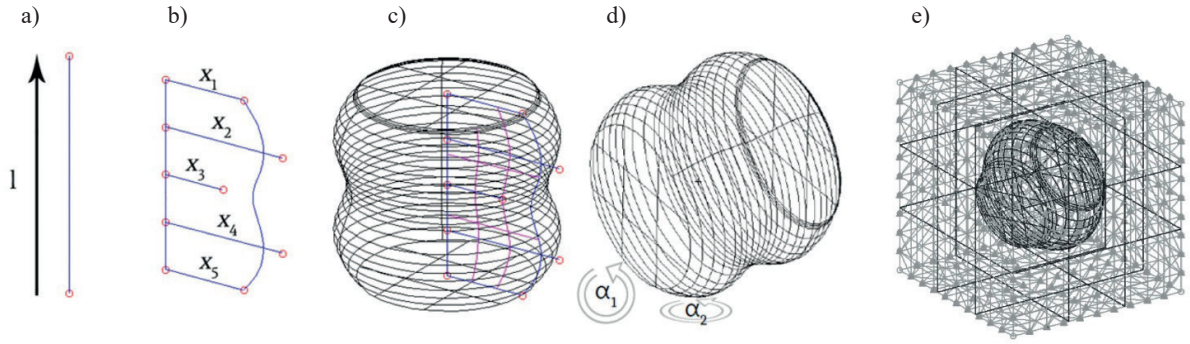

Fig. 3. Modelling of the RVE – design variables and discretization of the RVE:
a)-d) the subsequent steps of creating the geometry of the void; e) discretized RVE

Results for this example were obtained after solving approximately 10,000 boundary value problems and consist of a set of 100 Pareto-optimal (non-dominated) solutions found during the course of optimization. Values of objective functions for the obtained solutions are shown in the figures in two ways. A 3D scatter plot with values of the f_2 function represented by colour, and the remaining fitness function as values on the axes is shown in Figure 4. Scatter plot matrix of obtained solutions is shown in Figure 5. Along the diagonal are histogram plots of objective function values. On the basis of the presented plots of non-dominated solution some conclusions on the relationships between objectives can by drawn. On the 4D (3D + colour) plot, the solutions are arranged approximately in line, which indicates the existence of a degenerate real Pareto front in the problem. Looking at the scatter plot matrix, it can be noticed that this is caused by solutions displaying a similar nature pairwise.

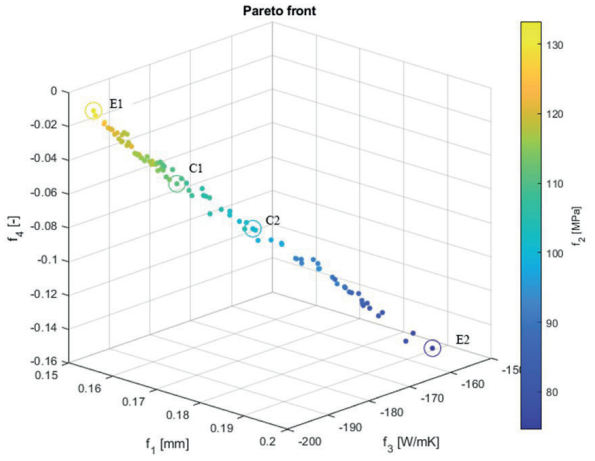

Fig. 4. Three-dimensional obtained Pareto-optimal solutions with f_2 criterion in color scale

Pairs of solutions in this example are proportional ($f_1 - f_3$ and $f_2 - f_4$) or inversely proportional (all remaining pairs). Examining the physical nature of the considered objectives, such a situation can be explained. For solutions in which the size of the pore was small, the thermal conductivity and stiffness were increased and therefore, values of optimization functionals f_1 and f_3 improved, which, however stand in conflicting nature of objectives related to volume and equivalent stress in the model, expressed in functionals f_2 and f_4. In general, it might be possible to find solutions with a low value of both objectives which should come in an agreement. Such a scenario is possible due to areas of increased stress concentration existing in the micromodel – pore of low volume, even though, usually results in low stress level, might in the case of specific shapes, exhibit locations of stress concentration. Nevertheless, such solutions are not interesting from the optimization point of view as they are dominated by other solutions in the solution space.

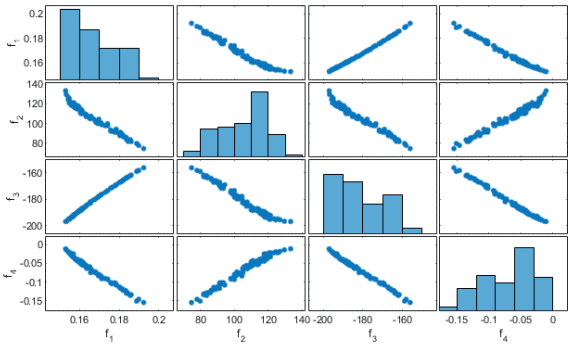

Fig. 5. Scatter plot matrix of obtained solutions

Among the found solutions, some solutions were highlighted. Solutions displaying extreme values of objectives f_1 and f_3 (E1), f_2 and f_4 (E2) as well as two compromise solutions (C1 and C2) are presented in detail. The geometry of these solutions is shown in Figure 6, and the values of objective functions and design variables are in Table 3.

Table 3. Values of fitness functions and design variables of selected solutions

Design	E1	E2	C1	C2
f_1 [mm]	0.152926	0.19227	0.162077	0.170551
f_2 [MPa]	133.239	74.6041	110.688	99.7959
f_3 [W/(m·K)]	−196.962	−156.136	−186.349	−176.84
f_4 [–]	−0.0109179	−0.154978	−0.0559121	−0.0838825
l [μm]	0.2543	0.5926	0.2365	0.3875
x_1 [μm]	0.093	0.3076	0.329	0.2941
x_2 [μm]	0.165	0.3437	0.3301	0.343
x_3 [μm]	0.1092	0.3335	0.3454	0.0925
x_4 [μm]	0.1047	0.1397	0.1448	0.3018
x_5 [μm]	0.1437	0.3241	0.1708	0.3064
α_1 [°]	88.4619	42.3712	22.1711	1.8684
α_2 [°]	48.3682	76.4589	89.3652	32.425

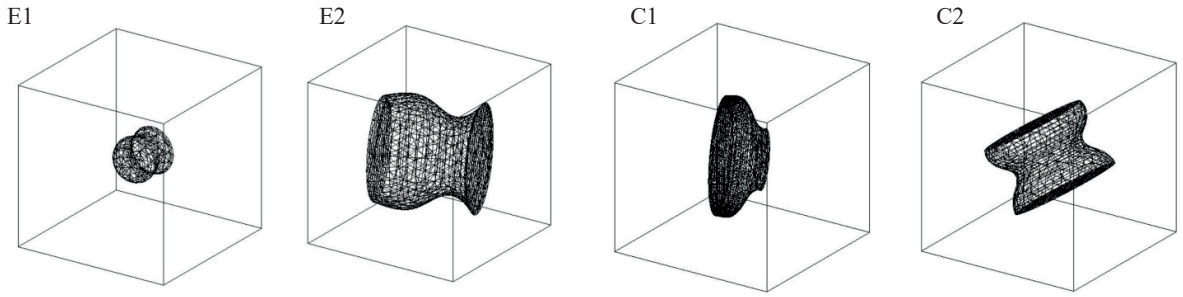

Fig. 6. Geometry of selected solutions

6. Final remarks

Multiobjective optimization of porous material in the multiscale was presented. Optimization of the geometry of microstructure was solved for four different proposed functionals. More functionals related to the particular needs asked of a porous structure can be formulated. A set of 100 non-dominated solutions was found. Proposed methods of visualisation help to draw conclusions on the natures of the objectives. Among the found solutions, some designs related to the extreme value of optimization functions were highlighted, compared in terms of design variables and the geometry of these solutions was shown. Analysing the relationships between non-dominated solutions and the shape of the Pareto front for the problem defined and solved in the paper, it appeared that the obtained set of solutions does not show more complex relationships, such as non-convexity or discontinuity of the front. In such a case, of course, the use of other less computationally expensive multi-criteria optimization methods can be considered, while this is not known apriori. In general, with a change of assumptions, i.e. a different definition of design variables, constraints, the consideration of additional criteria, etc., the situation can be quite different. It can be concluded that the developed method shows greater universality in comparison to traditional methods and its application can improve the multiscale design of porous systems.

Funding acknowledgment

The research was partially funded from the financial resources from the statutory subsidy of the Faculty of Mechanical Engineering, Silesian University of Technology.

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