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The comparative analysis of 2D and 3D microstructural models stresses of porous polymer materials

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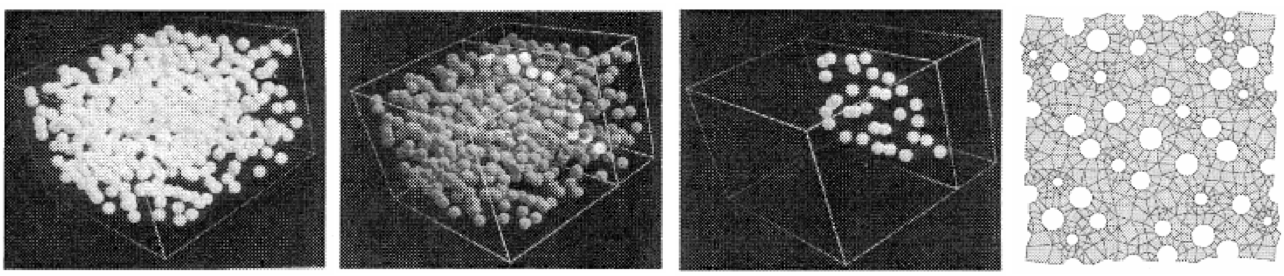
1. Introduction

Porous structural materials are widely used instead of monolithic these, because they are cheaper, lighter and exhibit good strength and deformability [1]. The spectrum of porous materials is very wide. They can be made from polymers (glassy, semi crystalline, elastomeric), metals (aluminium, nickel, copper), ceramics [1, 2 - 6]. These materials, components and products of them are widely used in the automotive industry, aviation, packaging, furniture, sewing, footwear trades. They have many fields of applications, including the manufacturing of thermal insulation, building materials, devices of buoyancy, absorbers, various filters, hydrophobic membranes, artificial leathers, shoes soles and a lot of others products [1, 7 - 11].

Porous material is a heterogeneous system with complex microstructure [12]. This system is diphase composite with solid matrix and gasiform filler [13, 14]. To determine the macroscopic overall characteristics of heterogeneous media is an essential problem in many engineering applications [15]. From the time and cost viewpoints, performing straightforward experimental measurements on a number of material samples, for various phase properties, volume fractions and loading histories is a hardly feasible task. On the other hand, due to the usually enormous difference in length scales involved, it is impossible, for instance, to generate a finite element mesh that accurately represents the microstructure and also allows the numerical solution of the macroscopic structural component within a reasonable amount of time on today's computational systems. To overcome this problem several homogenization methods have been developed to obtain a suitable constitutive model to be inserted at the macroscopic level [16 - 25]. Most of these methods are based on the concept of a representative volume element (RVE) [15]. The homogenized material properties are determined by fitting the results of the detailed modelling of the RVE (typically performed by the finite element method) on macroscopic phenomenological equations. The material configuration to be considered is assumed to be macroscopically homogeneous (continuum mechanics theory is suitable to describe the macroscopic behaviour), but microscopically heterogeneous. The physical and geometrical properties of the microstructure are identified by the RVE. It must be assumed that the structure of local microscopic material can be considered as the RVE surrounded by copies of itself, without overlapping of the RVEs and without voids between the boundaries of the RVEs. The RVE should be large enough to represent the microstructure, without introducing non-existing properties and at the same time, it should be small enough to allow efficient computational modelling [15].

Commonly a construction of RVE of heterogeneous system is performed in a simplified way, i. e. by the generation of 2D microstructural model or RVE instead of 3D this. Such procedure is illustrated in Fig. 1, where the construction of 2D RVE from 3D model is presented. Therefore, if the same assumptions are made the possibility of certain inaccuracy comes into existence. Same sources propose that the result of solved 2D problem shows a clear tendency of the 3D problem result [28]. It is obvious that the solution of 2D problem is both simpler and cheaper compare to 3D this. Therefore, the differences of the results obtained for 2D and 3D RVEs are not presented in any study. So the question about the suitability of 2D models use in any case arise.

The aim of this study was to investigate the stresses of 2D and 3D RVEs of porous polymer material, compare them and evaluate the differences between them in the cases of various porosity modes.



a b c d

Fig. 1 Construction of 2D RVE filed with voids: filing a cube with mono-sized spherical voids (a); define a 2D cutting plane (b); isolate the intersecting voids (c); mesh the cutting plane (d) (reproduced from Hall [26] and Smit [27])

2. Modelling

In order to investigate the stresses of 2D and 3D RVEs of porous polymer material and compare them, the computational studies were performed. The code ANSYS for finite element analysis (FEA) was used. Two cases of porosity mode were chosen and two types of 2D and 3D models were designed. The obtained models are over-simplified representation of porous materials structure, which was observed in many natural or artificial composite materials.

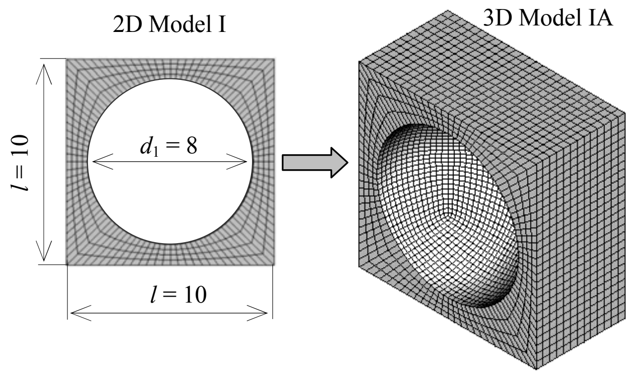


Fig. 2 Investigated 2D and 3D RVEs of first type models. 3D RVE is symmetrical and only half of it is shown. Dimensions are in μm

The first type models (2D Model I and 3D Model IA) were designed with one-sized pores with diameter d_1 and the distribution of them was somewhat periodical. The RVEs of this type models were assumed to be a square and a cube with a circle and a sphere in the centre respectively for 2D and 3D RVEs (Fig. 2). The cross-section of 3D RVE is identical to 2D RVE of Model I.

The second type models representing the other porosity mode were created on the basis of the first type these: smaller pores with diameter d_2 were added into the interpores zones. A distinct from the first case, the second type 3D models can be designed in more ways than one. Four 3D RVEs with the same cross-section identical to 2D RVE are presented in Fig. 3. These 3D RVEs are named as IIA, IIB, IIC and IID. Model IIA has additional pores d_2 only in the so-called main cross-section, which is shown. Model IIB was designed with additional pores d_2 in two cross-sections: the main one and the vertical perpendicular to this one. Model IIC was designed with additional pores d_2 in two cross-sections also: the main one and the horizontal perpendicular to this one. Finally, Model IID was created with additional pores in all three perpendicular cross-sections.

Eight-node quadrilateral PLANE183 (Structural Solid) elements with plane strain option were used for 2D models. Twenty-node brick SOLID 183 (Structural Solid) elements were used for 3D models. The exact number of the elements of each RVE depends on the model. It was approximately 200 and 50 000 elements respectively in 2D and 3D models.

The boundary conditions on the macroscopic scale were that the upper surface is shear-free with a constant displacement constraint; the bottom surface had constraint on two directions at the point on the symmetry axis of the model and on one direction in the other points. Whereas the right and left surfaces were assumed to be stress free. The total relative strain was 0.2. The case of small strains and linear dependence between stress and strain instead of non-linear this used for polymeric materials mostly were chosen due to the more acceptability of this case for the determination of stress concentration and stress concentration zones.

Mechanical properties of the material were typical for soft porous polymer material matrix. This group of materials was chosen due to the studies of these materials performed before [29, 30]. Young's modulus of matrix material was $E = 2.67$ MPa and Poison's ratio was $\nu = 0.48$.

Under the FEA performing the stresses of von Mises of 2D RVEs and 3D RVEs in the main cross-section were determined.

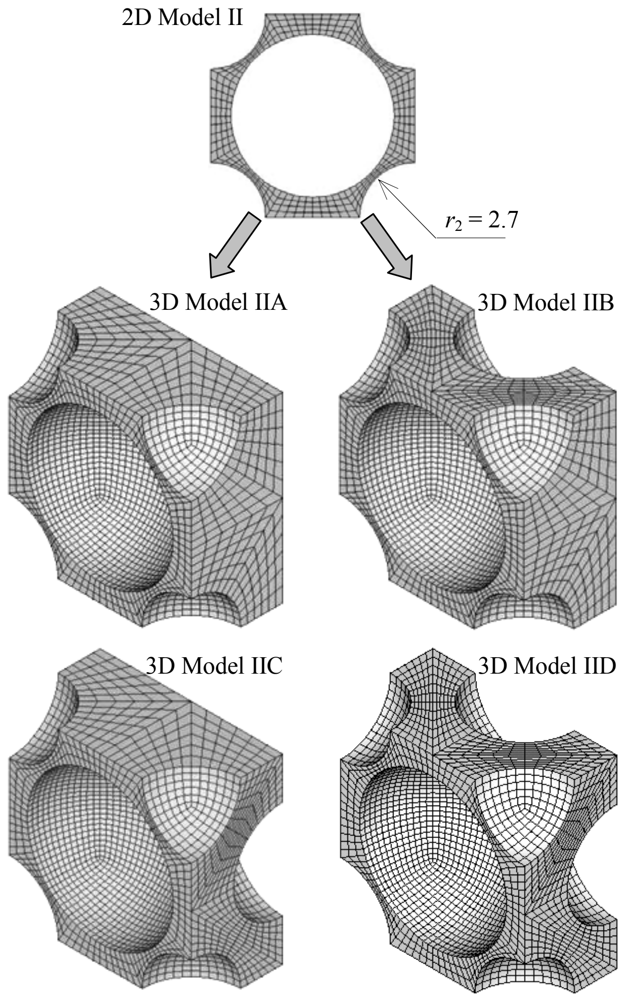


Fig. 3 Investigated 2D and 3D RVEs of second type models. 3D RVEs are symmetrical and only half of them is shown. Dimension is in μm

3. Results and Discussion

The von Mises stresses of 2D RVEs and 3D RVEs main cross-section are presented in Fig. 4. It seems that, the main tendency of the high stress of the first type models and the lower stress of the second type exist in both 2D and 3D cases. The stress of 2D Model I is about 2.3 times higher than that of 2D Model II. In the case of 3D models, the stress of the first type RVE is about 2 times higher than that of the second type. Therefore, it is evident that the result of solved 2D problem shows a clear tendency of the 3D problem result. However, the complete agreement of the results was not observed and the differences of 2D and 3D RVEs stresses were obtained.

In the case of the first type models it was calculated that the difference between stresses of 2D and 3D RVEs is equal to 8.7 %. In the case of the second type models the differences between stresses of 2D and 3D RVEs are presented in Table. It seems that, the stress differences between 2D RVE and 3D IIA, IIB RVEs are low enough and do not exceed 7 %. But from the comparison of the stresses of 2D RVE and 3D IIC, IID RVEs it seems that the difference is equal to 17 % and 13 % respectively.

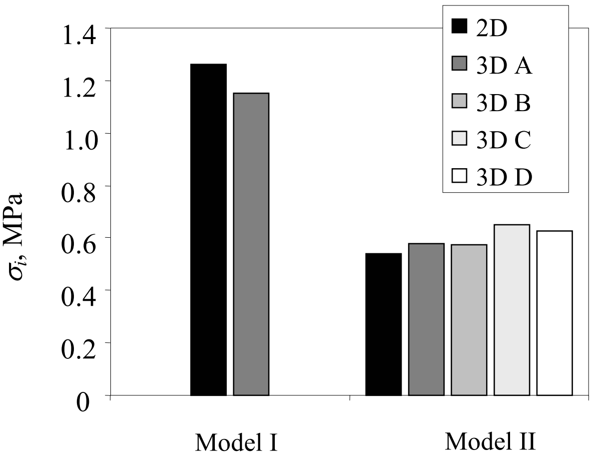


Fig. 4 The von Mises stresses of 2D RVEs and 3D RVEs main cross-section

The value of the difference depends upon the influence of additional pores in the deeper layers of 3D RVE. In the case of first type model, 2D RVE represent 3D RVE very exactly and the difference between stresses is low. How it seems, the presence of additional pores in some models of second type is not shown in the plane RVE.

Table

Comparison of stresses of the second type 2D and 3D RVEs

σ_i of 2D model, MPa	3D Model	σ_i of 3D model, MPa	$\Delta = \frac{\sigma_{3D} - \sigma_{2D}}{\sigma_{3D}} \cdot 100$, %
0.540	A	0.577	6.41
	B	0.573	5.85
	C	0.651	17.0
	D	0.624	13.5

The stresses of the second type 2D Model II and 3D Models IIA, IIB are comparable, thus these 3D models can be correctly described by 2D model. Nevertheless, 3D Models IIC and IID can not be precisely described by 2D model due to the difference higher than 10 %. The additional pores in the horizontal cross-section are characteristic for these models. These pores have a big influence on the stress state of 3D RVEs because they form the thin matrix strips (Fig. 5). The orientation of these thin strips is parallel with loading direction and as it is known from earlier studies [29], the presence of such strips cause the high stress concentration in them. Due to this, the stress state of 3D RVEs is changed and it can not be quite defined by 2D RVE.

As a result, what type of RVE either 2D or 3D is to be chosen depends upon the solved problem and pores distribution mode. If 2D RVE exactly represents the 3D model, the rigorous prediction of bulk material deformation behaviour could be done using 2D RVE. Nevertheless, if 2D RVE roughly defines all geometric properties of 3D model, only the tendency of stress distribution and the value could be evaluated in 2D RVE.

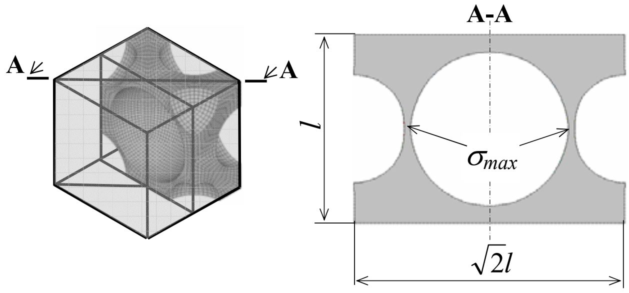


Fig. 5 Diagonal cross-section of Model IID RVE in which the stress is maximal

4. Conclusions

The stresses of 2D and 3D microstructural models of porous soft material were obtained and compared. The result of solved 2D problem showed a clear tendency of the 3D problem result. However, the complete agreement of the results was not observed.

If 2D model represents well the geometric properties of 3D model and there are no additional pores in 3D RVE, the influence of which can change the overall stress state of it, the rigorous prediction of deformation behaviour of volumetric material could be done using 2D RVE. The difference between stresses of 2D and 3D RVEs does not exceed 10 % in this case.

If 2D RVE roughly defines all geometric properties of 3D model, only the tendency of the stress distribution and the value could be evaluated in 2D RVE because the difference between stresses of 2D and 3D RVEs can exceed 10 %.

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PORINGŲJŲ POLIMERINIŲ MEDŽIAGŲ PLOKŠČIŲJŲ IR TŪRINIŲ MIKROSTRUKTŪRINIŲ MODELIŲ ĮTEMPIŲ LYGINAMOJI ANALIZĖ

R e z i u m ė

Baigtinių elementų analizės metodu buvo tiriami minkštųjų poringųjų polimerinių medžiagų plokščiųjų ir tūrinių mikrostruktūrinių modelių, apkrautų pastovia deformacija, įtempiai. Norint nustatyti, ar visais atvejais tūriniai modeliai gali būti pakeisti plokščiaisiais, kaip tai daroma daugelyje mokslo darbų, siekiant supaprastinti sprendžiamą uždavinį, buvo palyginti tūrinių ir jų pjūviams identiškų plokščiųjų mikrostruktūrinių modelių įtempiai. Nustatyta, kad plokščiojo uždavinio sprendimas parodo gana tikslias tūrinių modelių įtempių pasiskirstymo pjūvyje tendencijas, tačiau rezultatai nevisiškai sutampa. Jei plokščiasis modelis tiksliai atspindi tūrinio modelio geometrines savybes, galima pakankamai tiksliai prognozuoti tūrinės medžiagos elgseną. Šiuo atveju plokščiojo ir tūrinio modelių įtempiai skiriasi mažiau kaip 10 %. Tačiau jei tūriniame modelyje yra tokių porų, kurių įtaka įtempių būviui neįvertinama plokščiajame modelyje, t. y. plokščiasis modelis

neapibrėžia visų tūrinio modelio geometrinių savybių, tuo atveju, sprendžiant plokščiąjį uždavinį, galima nustatyti tik įtempių dydžio ir pasiskirstymo tendencijas, nes įtempių skirtumas gali viršyti 10 %.

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THE COMPARATIVE ANALYSIS OF 2D AND 3D MICROSTRUCTURAL MODELS STRESSES OF POROUS POLYMER MATERIALS

S u m m a r y

Finite element simulations were performed to study the stress state of 2D and 3D microstructural models of porous soft material under tensile loading by constant strain. The differences of stresses of 2D RVEs and 3D RVE cross-section identical to 2D RVE were obtained. The results showed that the solution of 2D problem provides a clear tendency of 3D problem solution. However, the quite complete agreement of the results was not observed. If 2D model represents well the geometric properties of 3D model, the rigorous prediction of deformation behaviour of volumetric material could be done using 2D RVE. The difference between stresses of 2D and 3D RVEs did not exceed 10 % in this case. If 2D RVE roughly defines all geometric properties of 3D model, only the tendency of the stress distribution and the value could be evaluated in 2D RVE because the difference between stresses of 2D and 3D RVEs can exceed 10 %.

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СРАВНИТЕЛЬНЫЙ АНАЛИЗ СОСТОЯНИЯ НАПРЯЖЕНИЙ ПОРИСТЫХ ПОЛИМЕРНЫХ МАТЕРИАЛОВ С ПРИМЕНЕНИЕМ ДВУХМЕРНЫХ И ТРЕХМЕРНЫХ МОДЕЛЕЙ МИКРОСТРУКТУРЫ

Р е з ю м е

Выполнен анализ состояния напряжений пористых полимерных материалов с применением двухмерных и трехмерных моделей микроструктуры и конечных элементов. Чтобы установить, во всех ли случаях трехмерные модели микроструктуры можно заменить более простыми, двухмерными, были сопоставлены между собой результаты состояния напряжений этих моделей. Установлено, что решение задачи с использованием плоского состояния напряжений достаточно точно описывает поведение объема материала в трехмерной модели. Если двухмерная модель точно описывает геометрию трехмерной модели, тогда можно достаточно точно прогнозировать поведение материала всего объема. В этом случае разница между напряжениями двухмерной и трехмерной модели не составило более 10 %. Однако, если в трехмерной модели имются такие поры, которые неучтены в двухмерной модели, то есть двухмерная модель не описывает всю геометрию трехмерной модели, тогда, решая плоскую задачу, можно судить только о тенденциях распределения напряжений. В таком случае разница между напряжениями двухмерной и трехмерной модели может превышать 10 %.

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