

NUMERICAL CALCULATIONS OF RVE DIMENSIONS FOR TWO-PHASE MATERIAL

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Abstract

A representative volume element (RVE) is a statistical representation of typical material properties. It should contain enough information on the microstructure thereby be sufficiently smaller than the macroscopic structural dimensions.

The paper deals with the numerical calculations of the dimensions of the RVE for a two-phase material microstructure. Two and three dimensional models are taken into consideration. The structure of the samples are developed on the base of randomization of elements belonging to one of the phases. The phases volume share is 50/50%. The following series of the models are analyzed: from 10 x 10 to 100 x 100 elements for 2D samples and from 10 x 10 x 10 to 100 x 100 x 100 elements for 3D samples. The element characteristic dimension is 10 μm . The elastic behavior of the base materials (magnesium and alumina) is taken into account. The quasi-static compression tests of the developed structures are carried out with the use of LS-DYNA computer code. The results are presented as the equivalent Young modulus values and compared to the calculations based on the rule of mixtures. The stabilization of the achieved results allows to assess the dimensions of the RVE for two-phase material with random distribution.

Keywords: *microstructure, two-phase material, metal-ceramic composite, RVE*

1. Introduction

Modern ceramic materials are currently the most often subject of materials science research because of their special properties, such as low relative weight, high hardness, specific damage mechanism (micro cracks propagation). These properties influence the energy absorbing and dispersion capabilities, that can be increased by using foamed materials, especially the ones with an open-cell structure, that can be infiltrated with other material (metal or elastomer). They are so called hybrid materials.

The manufacturing processes of those materials usually consist of the following three steps:

- Lay-up and fixation of the fibers, shaped as the desired component,
- Introduction of the matrix material,
- Final machining and, if required, further treatments like coating or generation of porosity.

In step one the fibers, often named rovings, are arranged and fixed using techniques applied in fiber-reinforced plastic materials, such as lay-up of fabrics, filament winding, braiding and knotting. The result of this procedure is called fiber-preform or simply preform. The third and final step of machining has to be done with diamond tools: grinding, drilling, lapping or milling. The special properties of the describe materials also allow to cut them with a water jet or a laser.

For the second step, five different procedures are used to fill the ceramic matrix in between the fibers of the preform:

- Deposition out of a gas mixture,
- Pyrolysis of a pre-ceramic polymer,
- Chemical reaction of elements,

- Sintering at low temperatures (1000 to 1200°C),
- Electrophoretic deposition of a ceramic powder.

The fifth procedure is not yet established in industrial processes. All procedures have sub-variations, which differ in technical details. Combinations of these procedures are also possible and applied.

The paper deals with the numerical calculations of the dimensions of the RVE for such two-phase material microstructure.

2. Two –phase materials modeling methods

The numerical models of materials and constructions allow to analyze complex phenomena, to assess the material properties, micro- and macrostructural strength behavior, energy absorbing capabilities. The simulations for static and dynamic processes with consideration of large deformations, contact, damage processes, heat transfer, strain rate effects are possible.

Various techniques and methods are used for the purposes of numerical modeling of foamed and composite materials. Numerical models may be developed on the base of the real structure image e.g. 2D photograph (Fig. 1) or 3D scan (Fig. 2). The 3D scans are obtained by use of X-ray or neutron tomography technique. Models may have a smooth shape or may be based on a grid technique. Idealized models are also often used for investigations of influence of particular geometrical or material parameters onto global properties of foam. They may be built on the base of geometrical solids (i.e. Kelvin’s polyhedron) [7], composition of different polyhedrons, Weaire-Phelan 8-cell repeatable structure [1] or on the way of Voronoi 3D tessellation [4]. Idealized models may represent multi cell structures or may be reduced to repeatable fragment of geometry – single cell or its part, so they are convenient for fast comparative analysis of long series of differentiated models.

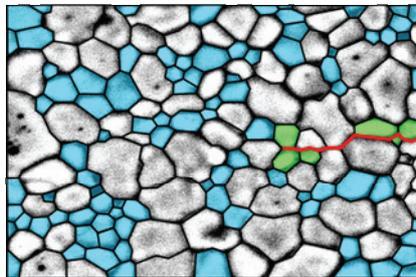


Fig. 1. Geometry of two-phase material real structure built on base of 2D photo [5]

The phenomenological models of materials may represent different levels of idealization. They are useful for the research of the structure geometry influence on properties of materials. The models can be two or three dimensional (Fig. 3 and 4).

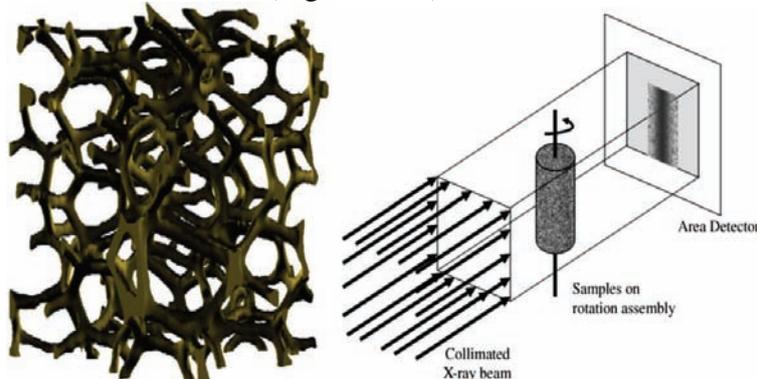


Fig. 2. Geometry of foamed material real structure built on base of 3D scan [3]

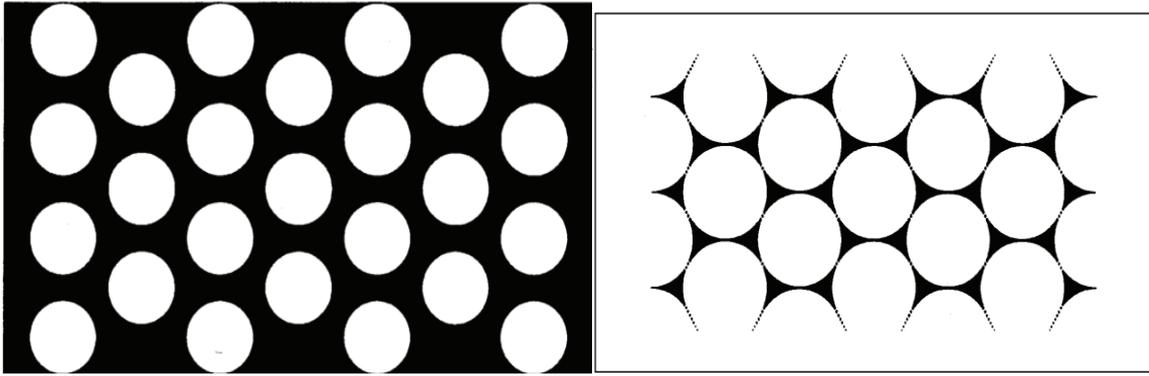


Fig. 3. Idealized two-dimensional geometry of foamed material structure [6]

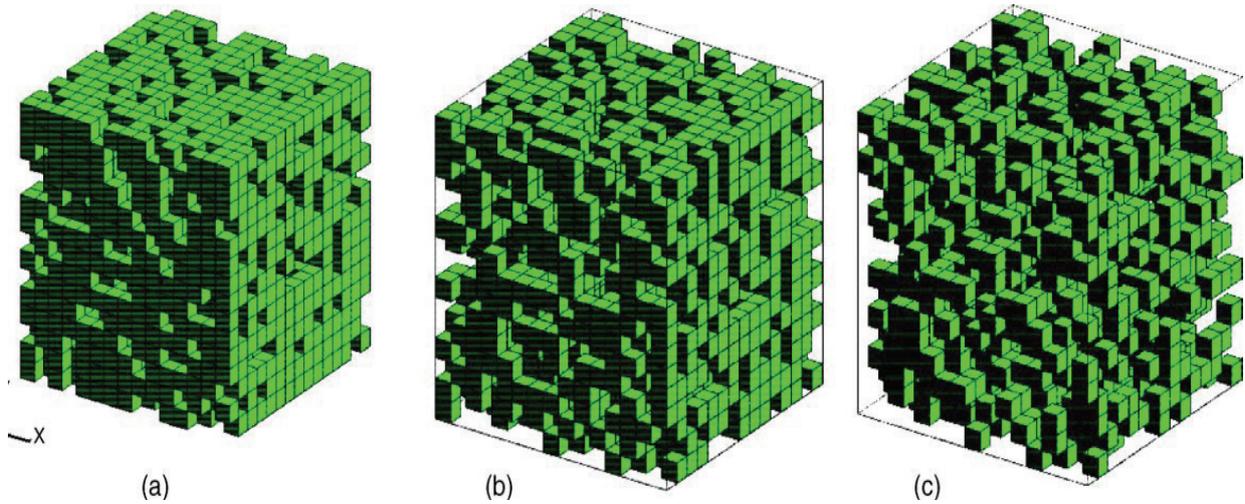


Fig. 4. Idealized two-dimensional raster geometry of foamed material structure [2]

The idealized models can also be generated on the base of size or shape and orientation of pores (Fig. 5 and 6). They are very useful for those factors influence research.

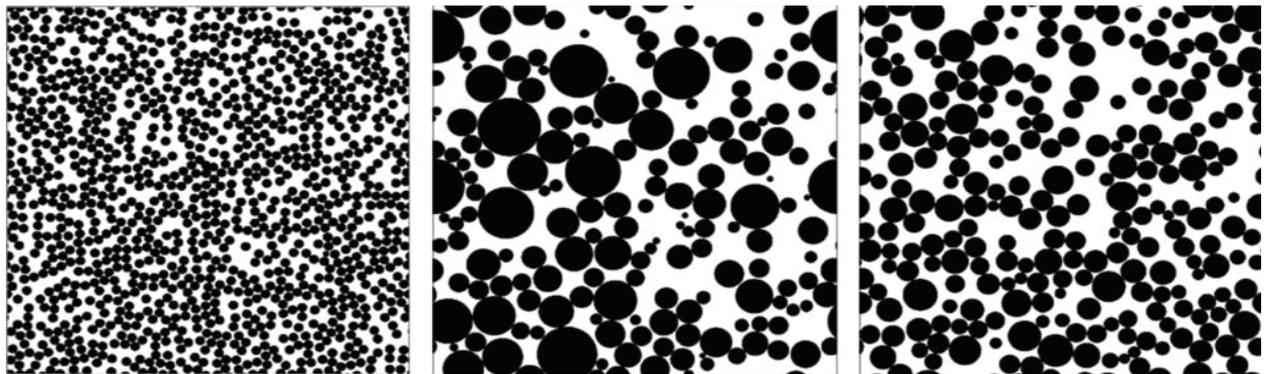


Fig. 5. Series of idealized models of foamed material structure considering pores size [6]

3. Representative Volume Element

The representative volume element (RVE) plays a central role in the mechanics and physics of random heterogeneous materials with a view to predicting their effective properties. A representative volume element (RVE) is a statistical representation of typical material properties. It should contain enough information on the microstructure yet be sufficiently smaller than the macroscopic structural dimensions [8] (see Fig. 6).

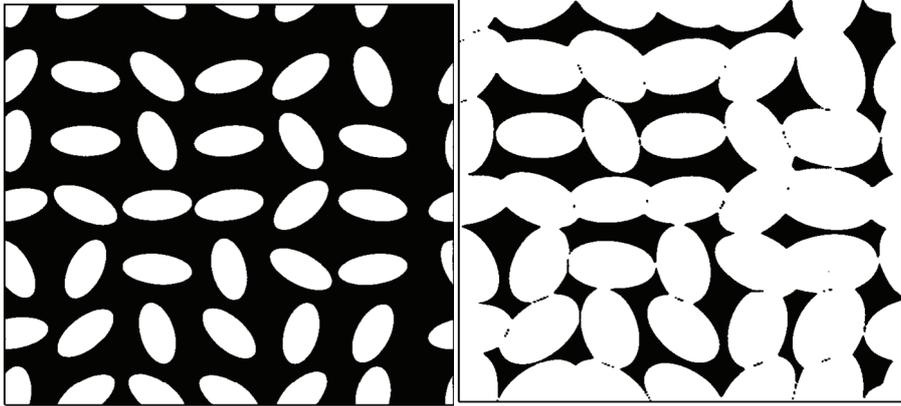


Fig. 6. Series of idealized models of foamed material structure considering pores distribution and orientation [6]

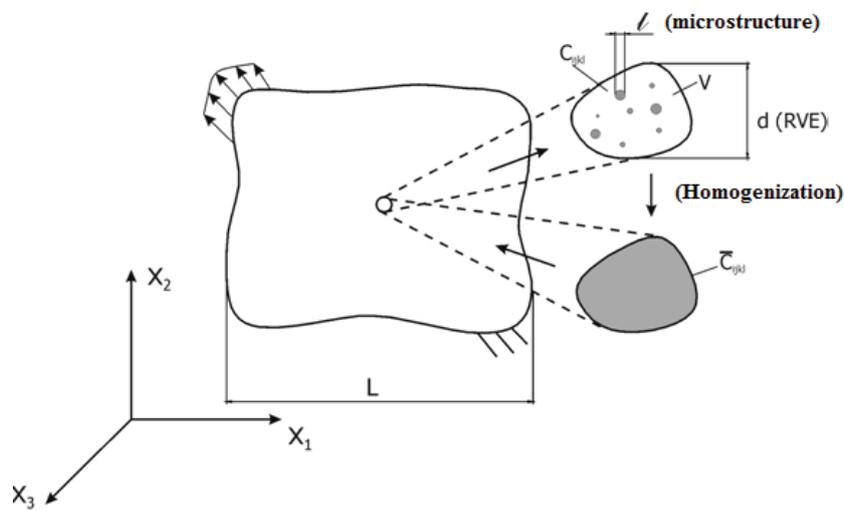


Fig. 6. Representative Volume Element

4. Numerical calculations of RVE for 2D and 3D models

The random raster numerical models of the two-phase material microstructure were developed for the purpose of the Representative Volume Element dimensions calculations.

The RVE assessment was carried out for the 2D models made of four-nodal shell finite elements and for 3D models made of eight-nodal solid finite elements. The series of the models that considered the dimension of the RVE were developed: 10 x 10, 20 x 20...100 x 100 elements (grains) and 10 x 10 x 10, 20 x 20 x 20...100 x 100 x 100 elements for 2D and 3D structures, respectively (Fig. 7-8). The percentage share of the phases was 50/50%. The element characteristic dimension is 10 μm . The phase elements distribution was realized by the randomization procedure that was carried out three times for each dimension.

The elastic behaviour of the base materials (magnesium and alumina) is taken into account. The material properties are as follows: $E_{\text{Mg}} = 45\text{GPa}$, $\nu_{\text{Mg}} = 0.29$, $E_{\text{SiC}} = 748\text{GPa}$, $\nu_{\text{SiC}} = 0.45$ (E – Young modulus, ν – Poisson ratio). The quasi-static compression test was carried out with the use of LS-DYNA computer code.

The results were presented as the equivalent Young modulus values vs. number of elements in the numerical model (Fig. 9-10). The regions of the results stability are visible in each case. The stability appears for the 2D model dimension of 80 x 80 elements and for 3D models – 40 x 40 x 40 elements.

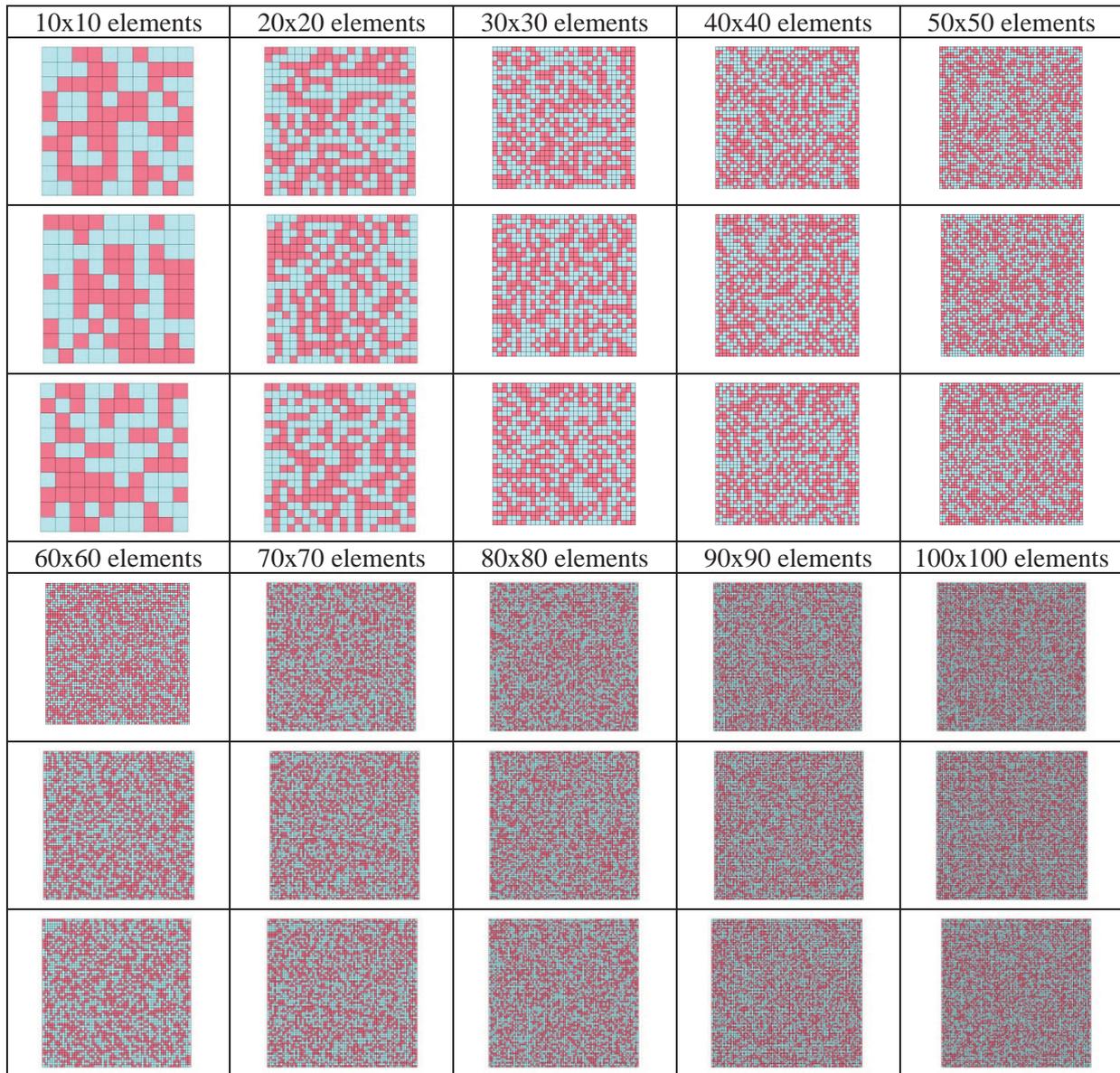


Fig. 7. Series of 2D models that consider the dimension of two-phase material RVE

The results presented above were compared to each other and with the results calculated on the base of the rule of mixtures, what is shown in Fig. 11.

The rule of mixtures allows calculating the average properties of the agglomerate in accordance to Eq. 1:

$$W = \sum_{i=1}^n X_i W_i, \tag{1}$$

where:

W - analysed material property,

X_i - fraction of phase i share,

W_i - analysed material property for phase i .

It can be concluded that the values for 2D and 3D models are the same for the sample dimensions of 80 x 80 elements and 40 x 40 x 40 elements, respectively. In both cases these values are about 10 MPa lower than calculated from the rule of mixture.

5. Conclusions

The numerical calculations of the dimensions of the RVE for a two-phase material microstructure were presented. Two and three dimensional models were taken into

consideration. The structure of the samples was developed on the base of randomization of elements belonging to one of the phases. The phase's volume share was 50/50%. The following series of the models were analyzed: from 10 x 10 to 100 x 100 elements for 2D samples and from 10 x 10 x 10 to 100 x 100 x 100 elements for 3D samples. The element characteristic dimension was 10 μm . The elastic behaviour of the base materials (magnesium and alumina) was taken into account. The quasi-static compression tests of the developed structures were carried out with the use of LS-DYNA computer code. The results were presented as the equivalent Young modulus values and compared to the calculations based on the rule of mixtures. The stabilization of the achieved results allows to assess the dimensions of the RVE for two-phase material with random distribution. The choice of the model (2D or 3D) must be based on the computational capacity of the available computer and time of analyses (30% shorter for 2D models).

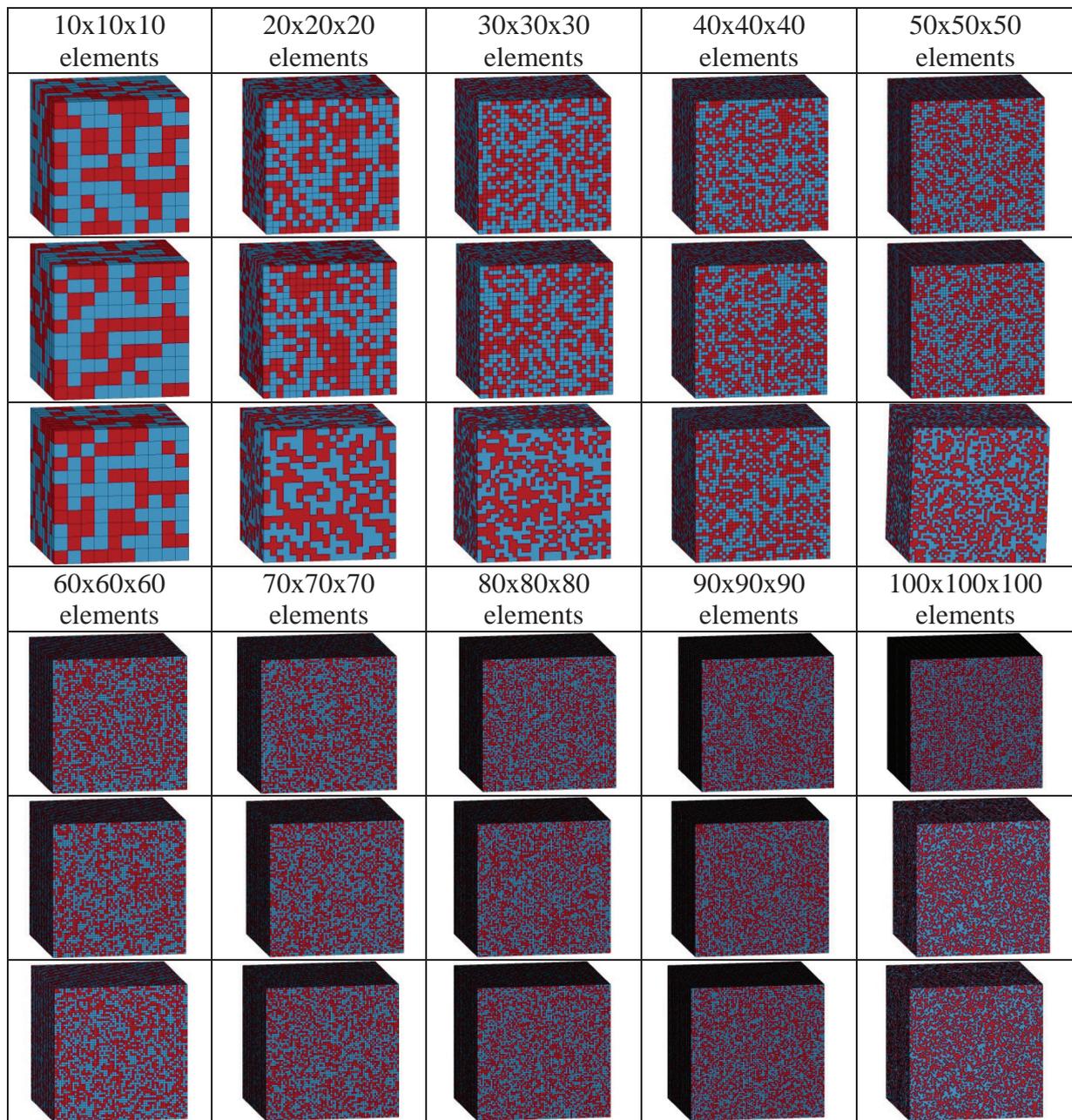


Fig. 8. Series of 3D models that consider the dimension of two-phase material RVE

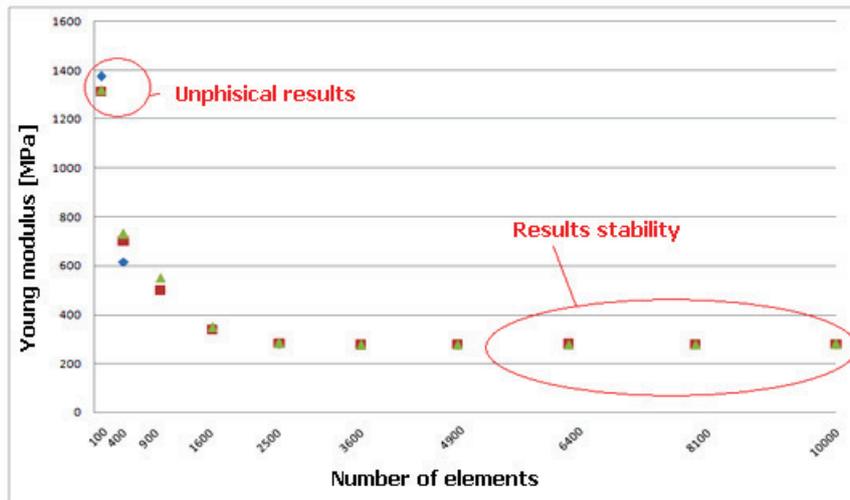


Fig. 9. Equivalent Young modulus values vs. number of elements in 2D numerical model

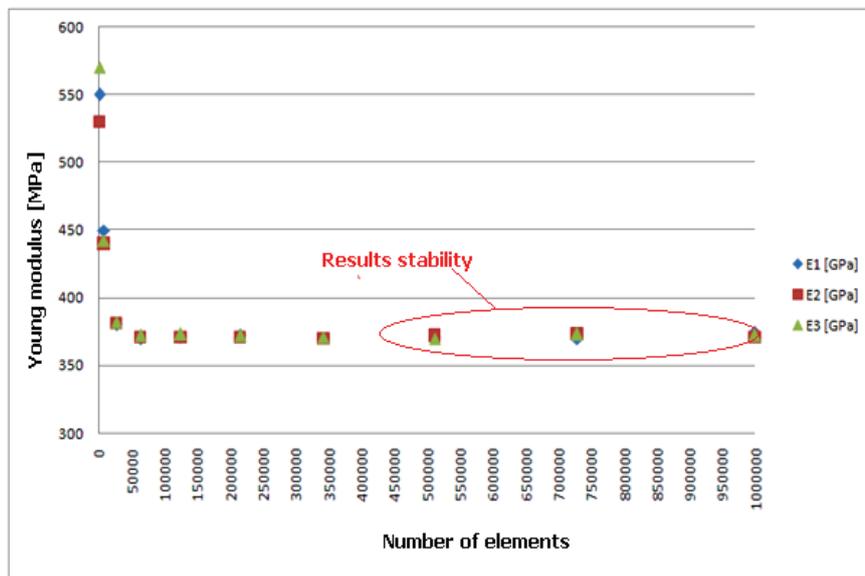


Fig. 10. Equivalent Young modulus values vs. number of elements in 3D numerical model

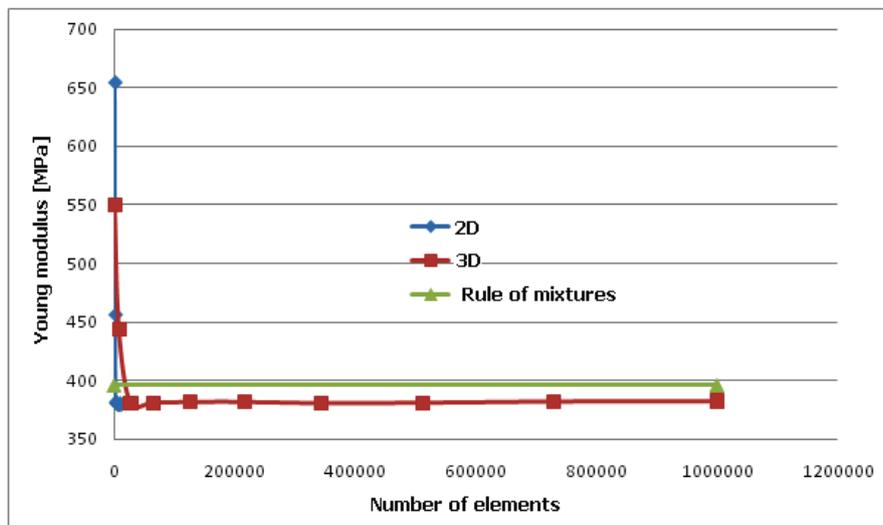


Fig. 11. Comparison of equivalent Young modulus values vs. number of elements for 2D and 3D numerical model and for rule of mixtures

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