OPTIMIZATION OF COMPOSITE MATERIALS WITH MATRIX AND SPHERICAL INCLUSIONS USING GENETIC ALGORITHMS

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***Abstract**. The computational mechanics is an important tool to make researches of the behavior of micro-heterogeneous materials, as the extensive literature on this issue shows. In a previous work written by the authors , a representative volume element (RVE) of a biphasic material formed by a spherical in-homogeneities, randomly embedded in linear elastic and isotropic matrix was determined. In the present work a regular distribution of in-homogeneities was considered, thus avoiding handling multiple samples. A Genetic Algorithm was used as a tool to optimize three Cases that are described as follows: Case A, where the determination of the in-homogeneities K and μ elastic constants, maintaining the properties of the matrix and the composite constant is proposed. Case B, where the best combination of real materials to create desired effective properties for the compound is searched, and finally Case C, where the determination of the in-homogeneities K and μ elastic parameters, keeping the properties of the matrix and the composite, trying to minimize the variation of stress in the compound is accomplished. In the conclusions, commentaries about the obtained results are done.*

***Keywords:** optimization, particulate composite, genetic algorithm, finite element method, micromechanics.*

1. INTRODUCTION

The increasing technological progress, especially in the engineering field, directly influences the design and production of new products using new materials in an effective way. In this context, the composite materials are highlighted, since the combination of two or more materials may generate advantageous properties when compared to a single material. The composite material concept allows engineers “to create” new materials through the combination of single materials components. To enhance or worsen some mechanical characteristics and avoid some failure modes, a computational optimization technique can be used. Several aspects of the behavior of the material can be handled in the design of a compound, such as: static and fatigue strength, stiffness, corrosion resistance, abrasion resistance, total weight, ability to work at high and low temperature, acoustic insulation, thermal conductivity, electric hardness, ductility and aesthetic appearance as seen in Mendonça (2005).

An example of application of compounds is the frequent use of polymer and materials of polymeric matrix in applications of high-precision engineering, with emphasis, in South America, for polypropylene (PP) and polymethylmethacrylate (PMMA), as can be seen in the sites of Argentinean Association of Plastic Industry (http://www.caip.org.ar) and the Brazilian Association of Plastic Industry (http://abiplast.org.br). Since material being studied is linear elastic and isotropic, its behavior can be characterized by the values of elastic constants K (Bulk modulus) and μ (shear modulus) of the homogenized composite material. In contrast, the non-linear mechanical behavior that can also be significantly modified with the in-homogeneities from the second phase requires more complex interactions.

To face this, the numerical computational modeling is an important ally in the search of the behavior of micro-heterogeneous materials. By the computational mechanics the relationship between the micro-structure and macro-structural properties of the material can be determined. In order to find the macroscopic constitutive behavior, it is necessary to perform a computational homogenization, which is a multi-scale technique. This is accomplished in the micro-structure level by constructing and solving a boundary element problem for the micro-structure.

Since calculations involve materials, database manipulation and sometimes discrete design variables, traditional optimization methods are not suitable as they use gradients of the optimization function. The lack of robustness of classical gradient based deterministic optimization processes can be overcome by application of Genetic Algorithms technique.

Thus, this work aims at performing an optimization using the Genetic Algorithms (GA) technique in the representative volume element (RVE) of thermoplastic polymeric matrix with spherical in-homogeneities of elastomers determined by Soares *et al.*, (2008). Specifically, it aims at: Case A: determine K and μ of the in-homogeneities keeping constant the properties of the matrix and K^* and μ^* for the compound; Case B search in a thermoplastic and elastomers' list, the best combination of materials to generate the desired K^* and μ^*; Case C determine K and μ of the in-homogeneities keeping constant matrix properties and minimizing the interface stresses between phases. The results found by this paper were satisfactory and the objectives were fully achieved.

2. THEORETICAL FUNDAMENTATION

2.1. Micromechanics

The problem to obtain the properties of a compound material out of the properties of material constituents is solved in the light of the Micro-Mechanics Theory. In the previous paper (Soares *et al.*, 2008), techniques of homogenization presented by Suquet (1985) and Zohdi (2002) were applied to compute the representative volume element (RVE) of a biphasic material composed by polymer matrix (PMMA) and spherical in-homogeneities (rubber) with random distribution . The elastic constants K and μ for the composite were taken as global parameters in this study to measure RVE.

Not only the matrix and in-homogeneities material properties, but also the compound ones with isotropic linear elastic behavior were considered. The process to determine RVE was carried out analyzing samples of the compound material with different amounts of micro-heterogeneities, computing global parameter (see expressions (1)) and observing their behaviors. RVE is the size of the sample that contains a minimum number of particles where the global parameters of the sample remained constant. In this study, five sizes of samples containing 2, 4, 8, 16 and 20 spherical in-homogeneities with random distribution in the matrix were analyzed, considering the average and dispersion of results, with different volume fractions for the nodular phase. The RVE for a 10% nodular volume fraction of the sample indicates samples with 8 in-homogeneities.

The elastic constants of the compound considered as global parameters were obtained through the equations below, taking into account the condition of Hill (Zohdi, 2002):

$$3K^* = \frac{\langle \frac{\mathrm{tr}\,\sigma}{3} \rangle_\Omega}{\langle \frac{\mathrm{tr}\,\varepsilon}{3} \rangle_\Omega} \qquad \text{and} \qquad 2\mu^* = \sqrt{\frac{\langle \sigma' \rangle_\Omega : \langle \sigma' \rangle_\Omega}{\langle \varepsilon' \rangle_\Omega : \langle \varepsilon' \rangle_\Omega}} \tag{1}$$

where $\frac{\mathrm{tr}\,\sigma}{3}$ and $\frac{\mathrm{tr}\,\varepsilon}{3}$ are the hydrostatic stress and strain and $\sigma' = \sigma - \frac{\mathrm{tr}\,\sigma}{3} I$ and $\varepsilon' = \varepsilon - \frac{\mathrm{tr}\,\varepsilon}{3} I$ the stress and strain deviadoric tensor, I is the identity matrix, σ ,and ε represent the stress and strain tensors, respectively. The symbol < . > represent an average operator, calculated component by component.

The values of expression (1) were calculated processing the results obtained by means of ABAQUS , a finite element commercial code.

Figure 1 show the RVE obtained in Soares *et al.*, 2008 study.

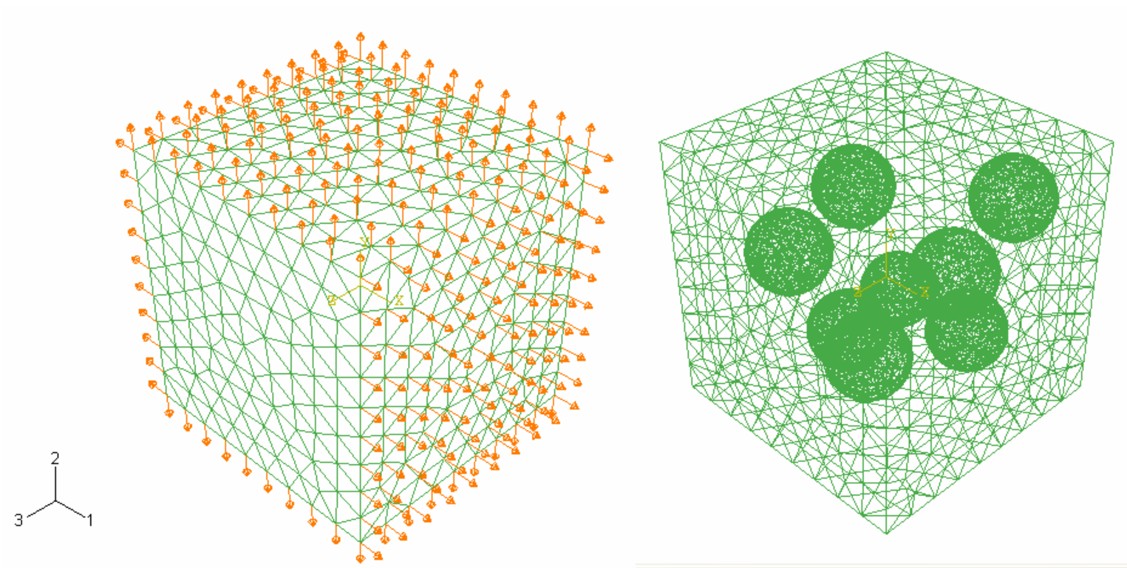

Figure 1: Mesh, boundary conditions and random distribution of 8 spherical nodules (RVE) of a sample used in the study by Soares *et al2008.*

2.2. Introduction to Genetic Algorithms Method

Genetic Algorithms (GA) is an optimization technique based on Darwin's Theory of evolution. The Darwin's Theory of Natural Selection says that "… any being, if it varies slightly in any manner profitable to itself, will have better chance of surviving…". GA simulates the evolutionary process numerically. They represent the parameters in a given problem by encoding them into a string. The genetics, genes are constituted by chromosomes. Similarly, in simple GA, encoded strings are composed of bits.

A string of bits can be decoded to the respective problem parameter value and the total evaluation of the bits string for an individual may be weighed following some fitness function representing the phenotype of the bits string.

A simple genetic algorithm consists of three basic operations, these are: reproduction, crossover and mutation. The algorithm begins with a population of individuals each of them representing a possible solution of the problem. The individuals, as in nature, perform the three basic operations and evolve in generations where the Darwin's Theory prevails, or in other words, a population of individuals more adapted emerges as natural selection.

At the reproduction level, the evaluation of the objective (fitness) function indicates which individuals will have more chances to procreate and generates a larger offspring.

In the genetic operations the genes of pair of individuals are exchanged and, as in nature, this may be performed by several ways, this operation is called crossover.

The basic differences between, stated by Goldberg (1989) between conventional techniques and the genetic algorithm (GA) can be summarized as follows:

- GA operates on a coded form of the parameters used in the optimization instead of the parameters itself;
- The GA works with a population which represents numerical values of a particular variable; differently from classical optimization algorithms which require objective functions evaluations and gradients.
- Only probabilistic rules of natural selection are used with GA.

The global convergence proof of GA can be found in the literature such as Zeng et al (2005) or Liepins (2002).

The algorithm starts generating a random set of individual that will form the population. In the following, individual are selected and picked on pairs according its fitness (objective function). This is accomplished by a probabilistic raffle called roulette wheel. At this point crossover will occur, mixing chromosomes from two individual generating two offspring with characteristics inherited from its parents. The reproduction will be promising with a probability 'Pc'. At last, from the offspring population, some chromosomes of some individual will suffer mutation under a probabilistic rate 'Pm' usually set as a low value (1% or less) as found in nature. Then, eventually, some best individual belonging to the parent set will bypass the natural selection and will be introduced in the offspring set through an elitism procedure and exchanged by the less fitted offspring. This procedure assures that best solutions are hold and not lost in the probabilistic selection. The generations will succeed until a convergence criterion being reached, such as the diversity on the population set evaluated by the standard deviation of the objective function (fitness).

3. CHARACTERIZATION OF STUDIED MODEL AND GENETIC ALGORITHM IMPLEMENTATION

3.1. Model

The RVE determined by Soares *et al.*, (2008), for nodules volume fraction of 10% over the volume of the sample implicated in 8 in-homogeneities, as already mentioned. The properties of the matrix are characterized by E = 3240MPa and $\nu = 0.25$, while the second phase material constant by E = 40MPa and $\nu = 0.40$, in this case the nodules were considered with the same radius.

In Soares *et al.*, (2008), because the model has linear elastic both phases and the second phase volume ratio is equal to 10%, a very little variation in terms of compound elastic constant was observed, when the random distribution of the nodules was changed. For this reason, in the present work a simplification in the model to be optimized, a regular distribution of in-homogeneities in the matrix was chosen to be accomplished. In this way the effort to handle with an average and dispersion of different random configurations was avoided.

Figure 2 shows the mesh and the regular distribution of the model to be optimized.

3.1. Genetic Algorithm Implementation

The main steps of the GA implementation used in the present work were summarized as follows:

1) The characteristics of interest in terms of chromosomes were codified.
2) For t = 0, the initial population B0 = (B10, B20, ...) with some diversity was assessed;
3) While the stop criterion wasn't accomplished , the follow procedures will be repeated:
   - Selection of individuals from the t-esim population Bt taking into account the probability of survival of better adapted, i.e. who individual has higher objective function.

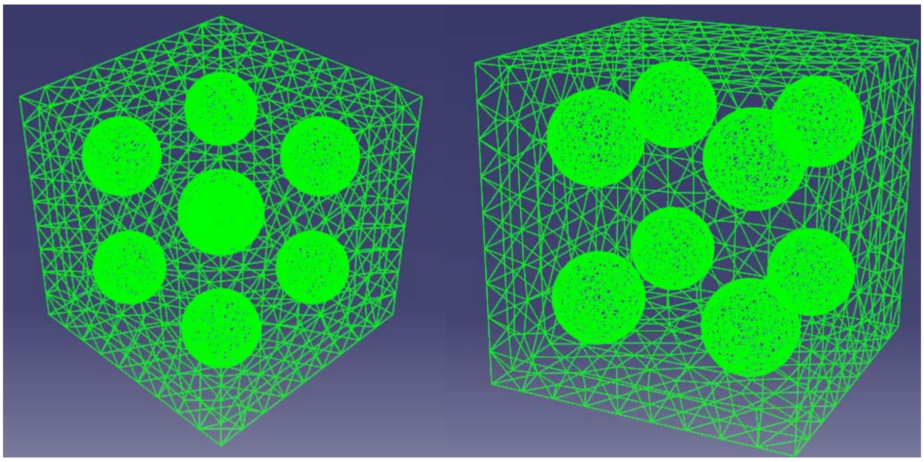

Figure 2: Mesh and regular distribution of 8 spherical nodules model studied.

- Generation of “offspring” hence the reproduction of these individuals are carried out using the Roulette wheel procedure.;
- The mutation of some of these individuals are sometimes made;
- The adaptation of the new generation Bt+1 according to the old previous generations is carried out.
- In the present implementation of genetic algorithms, the elitism has also been incorporated. That one produces individuals of higher performance be automatically selected. In this way, it is avoided that the genetic operators can make changes in this individuals.

-The stop criterion in the algorithm was the stationary state achieved by diversity.

Figure 3 shows the flow-chart of the genetic algorithm implementation.

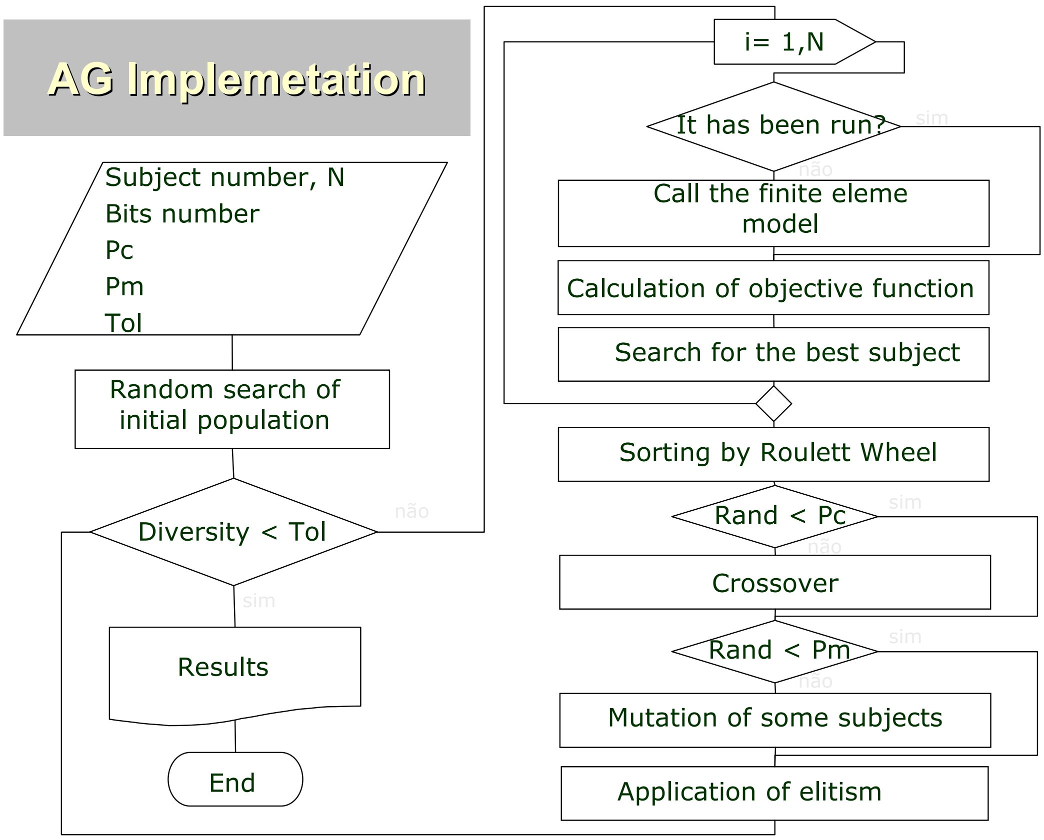

Figure 3: Flowchart of genetic algorithms implementation

4. RESULTS AND DICUSSIONS

In the models of the thermoplastic polymeric matrix with spherical elastomeric in-homogeneities an optimization using a GA was performed. The following examples were studied:

- Case A: In this case the determination of the in-homogeneities K and μ elastic constants, keeping the properties of the matrix and the composite is proposed.
- Case B: In this case the best combination of thermoplastic and elastomeric real materials (http://www.ndsm.ufrgs.br), to create desired effective properties for the compound, is searched.
- Case C: In this case the determination of the in-homogeneities K and μ elastic constants keeping the properties of the matrix and the compound constants and minimizing the variation of stress in the compound is accomplished.

4.1. Case A

In this case, the matrix properties was kept, leaving variable the in-homogeneities properties. The target compound properties were stipulated using the values obtained in the RVE study, accomplished by Soares *et al.*, (2008).

In this case the objective function (Fitness) to maximize, each individual i, was:

$$\text{Fitness(i)} = \frac{1}{1 + \frac{|K(i) - K^*|}{K^*} + \frac{|\mu(i) - \mu^*|}{\mu^*}} \tag{2}$$

When the differences between the K(i) and μ(i) and the target values K* and μ* reach a minimum value, this indicates that the best fitness value was achieved. The properties of the matrix are characterized by E_m = 3240MPa and νm = 0.25 and the compound material by: K*=1784,86MPa and μ*=1095,05MPa.

A data-base with all individual evaluated up this moment was built. In this way a rework is avoided, because GA, before evaluating a new individual, searches, in that data base, if its evaluation is there.

Table 1 presents the main data related to this case. The amount of bits used to define each variable, and the range of variation for a population of 20 individuals is presented. Others important parameters that have to be defined to implement a genetic algorithms scheme, they are: the probability of crossover (Pc) = 90%, the probability of mutation (Pm) = 10% and the maximum tolerance of the standard deviation of individual diversity (tol)= 1,0e-05.

Table 1: Number of bits and limits applied to study the variables of Case A.

Variable	Nº. bits	Lower limit	High limit
ν_i	5	0,0	0,5
E_i	9	1,0 MPa	4000,0MPa

The in-homogeneities properties obtained using the implementation of GA carried out for Case A were: E_i=47,955MPa and ν_i=0,403, closed values to the expected ones (E_i=40Mpa, ν_i=0,40, used in Soares *et al.*, (2008)).

The configuration shown in Table 1 would allow (2^9+2^5=16384) combinations of E_i and ν_i. Even if, in the present work, only 520 pairs of E_i and ν_i were necessary to evaluated using the GA implementation proposed, that is, in terms of the GA terminology, 26 generations of 20 individuals each one. However, by means of a database of all individuals evaluated in the optimization process, only 89 different ones (approximately 6 times less than the 520 individuals) were necessary to evaluated.

The present case lets us emphasize the advantage of GA implementation, once only 0,5% of all possible combinations of individuals (E_i and ν_i values) were evaluated to find the target result, in other words, from 16,384 possible combinations, only 89 ones were evaluated.

4.2. Case B

In case B the best combination of matrix and in-homogeneities materials to obtain a compound with elastic Young Modulus E* as target is searched. The in-homogeneities used in the compound have regular distribution and a volume concentration of (10%). The Matrix material is selected from 32 real thermoplastic materials and the in-homogeneities are selected from 8 possibilities, that is : 7 elastomers and a null material to simulate a cavity option. The elastic properties that characterize the Matrix and In-homogeneities option materials are presented in Table 2.

The Fitness function used in the present study is shown as follows:

$$\text{Fitness(i)} = \frac{1}{1+\frac{|E(i)-E^*|}{E^*}} \qquad (3)$$

The best combination of materials for the matrix and in-homogeneities will be the option that minimizes the Fitness(i) function shown in (3).

The target property for the compound is: E *= 2000MPa.

Table 3 presents the GA parameters defined in Case B.

Table 2: List of elastic properties used for the matrix and for in-homogeneities (http://www.ndsm.ufrgs.br)

THERMOPLASTIC MATRIX								
Material	**E(MPa)**	**ν**	**Material**	**E(MPa)**	**ν**	**Material**	**E(MPa)**	**ν**
1-ABS- High Impact	900	0,4	15-PI	4225	0,4375	29-Phenolic	6437,5	0,40625
2-ABS- Medium Impac	1350	0,4	16-PMMA	2150	0,4075	30-Phenolic	7312,5	0,41875
3-Nylon 11	925	0,4	17-PMMA	2850	0,4225	31-Phenolic	8187,5	0,43125
4-Nylon 6	2500	0,4	18-Hard Polyester	2975	0,4125	32-Phenolic	9062,5	0,44375
5-Nylon 6/6	2400	0,4	19-Hard Polyester	3925	0,4375	**ELASTOMER INHOMOGENEITIES**		
6-PBT	2150	0,375	20-PP	1987,5	0,425	**Material**	**E(MPa)**	**ν**
7-PC	2450	0,415	21-PPO	2287,5	0,375	1-Epdm	53,025	0,48375
8-PEAD	1200	0,41	22-PS	3100	0,415	2-Epdm	157,675	0,49125
9-PEBD	650	0,44	23-PTFE (teflon)	500	0,455	3-EVA	25	0,48
10-PEEK	725	0,405	24-PU	16	0,494	4-Isoprene	1,85	0,49925
11-PES	2650	0,4	25-PVC Rígido	3150	0,4	5-Neoprene	1,35	0,4925
12-PT	2525	0,3925	26-SAN	3175	0,385	6-SBR	6	0,488
13-PT	3175	0,4175	27-Alkydes	7500	0,4125	7-Hard Silicone	5,5	0,385
14-PI	3075	0,4125	28-Alkydes	8500	0,4375	8-Empty	1.0e-7	1.0e-7

Table 3: GA parameters defined in Case B.

Number of individuals	20
Variable 1	5 bits, matrix: 32 different materials (2^5)
Variable 2	3 bits, in-homogeneities: 8 different materials(2^3)
p_c	90%
p_m	10%
tol	1,0e-05

In the present case, for each individual evaluated, a finite element model with the matrix and in-homogeneities material properties selected must be computed.

Similarly with Case A, in the present Case a database with all individuals evaluated was implemented, but as the number of individuals evaluated was very little, the reduction in the number of evaluation was insignificant.

The best combination among the materials presented in Table 2 was the Polyphenylene Oxide (PPO), for the matrix and Ethylene Propylene Diene M-class rubber for the in-homogeneities, materials number 21 and 2 respectively in the list shown in Table 2. The elastic Young Modulus for the compound of these material combinations was E*=1994MPa, representing an error of 0,3%, regarding the desired value.

Among the materials shown in Table 2 , there are (2^5+2^3=256) possible combinations. With the implemented GA scheme of optimization, 319 generations and 130 different individual evaluations were needed. The optimum combination was found in the second generation, but to accomplish the diversity criterion imposed, it was necessary to compute the rest of evaluated individuals.

Observing these results in percentages, up to 50% of the possible combinations were needed to find the best individual(130 over 256 possible evaluations), but the optimum individual was found only with 13% of the possible combinations, that is 33 over 256 individuals.

Also the same Case, using 6 and 10 individuals in each generation were studied.

The obtained results are carry out in terms of number of individuals in each generation vs ratio between the combinations made over possible combinations, and the error committed in the estimative of E*.

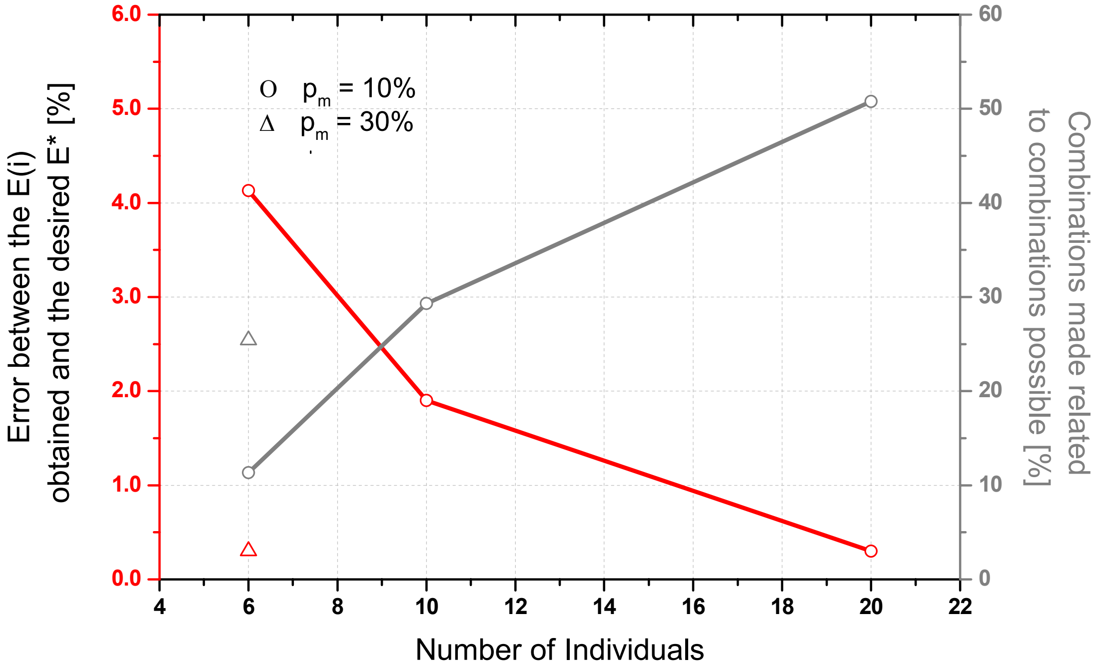

Figure 4: Influence of the number of individuals in each generation in terms of the ratio of the number of combination made over number of possible combinations in [%], and error in the estimative of E* in [%]

In Figure 4, it is possible to observe the ratio between made combinations over possible combinations that diminishes when the quantity of individuals in each generation diminishes. On the other hand, when the number of individual diminishes the error in the estimative of the E* grows.

If we grow the mutation probability from 10% to 30% for 6 individuals in each generation, the estimative error for E* drops from 4% to 0,3 %, but in compensation the number of combinations to be evaluated grows from 13% to 25% (see these values in the grey and red triangle dots in Figure 4).

As a last commentary, it is possible to add that other parameters such as density, toughness transition temperature, electrical conductivity, among others, might be taken into account. For example the best combination for the matrix and in-homogeneities materials could be searched to reach a target E*, with restriction of the in-homogeneities density of the compound.

4.2. Case C

In Case C the GA implementation consistence is demonstrated. The analyzed problem consists in determining the in-homogeneities properties, for fixed matrix properties that minimize the stress gradient in the compound material. It is easy to deduce that the best option for the in-homogeneities properties happens when the matrix and in-homogeneities properties are the same. In the present Case we aim at verifying if the implemented GA algorithm confirms this expected tendency.

In this way the fitness function to be maximized will be:

$$\text{Fitness(i)} = \frac{1}{1+\text{CV}} \tag{4}$$

Where CV represents the Von Mises stress coefficient variation, computed element by element overall the finite element model used.

In Table 1 the control parameters of GA algorithms for the present Case are shown, which results equal than the parameters adopted for Case A. Additional parameters control such as number of individuals, probability of crossover and mutation, and maximum tolerance of the standard deviation of diversity of individuals, also were set in the same way as Case A (Nindv=10, Pc=90%,Pm=10%, tol=1,0e-05).

The in-homogeneitiesand matrix properties were fixed adopting the same values used in Soares et al (2008), that is E_m=3240,ν_m=0.25, E_i=40Mpa, ν_i=0,40. The variation coefficient in terms of Von Mises Stress in the compound material are 58,12%.

The target in-homogeneities properties E_i=3201,77MPa and ν_i=0,2581, were obtained using the implemented GA algoritms. This result shows clearly the tendency of the -homogeneity in to adopt the same properties that the matrix.

In Figure 4a a cut in the used finite element model with the Von Mises stress map is shown. The properties used were the same of Soares et al (2008), that is, E_i=40Mpa, ν_i=0,40, E_m=3240MPa, ν=0.25. The Von Mises stress strip observed in the present case was from $3{,}369E^{-6}N/\mu m^2$ to $3{,}718E^{-4}N/\mu m^2$, obtaining a mean Von Mises Stress of $1{,}8474E^{-4}N/\mu m^2$. In Figure 4b1, a cut in the finite element model with optimized properties using the same map scale of Figure 4a was also illustrated. It is possible to observe in the last figure that no variation is perceived. Finally, in Figure 4b2 the cut in the model with optimized properties is depicted, but now with another Von Mises Stress Scale. A very little variation is identified in this case (CV=0.61%).

In the same way of the one in Case A, there are 16384 possible combinations of E_i and ν_i.

Using the GA implementation, it will be necessary to evaluate 1000 individuals in order to reach the optimized solution, using 49 generations with 20 individuals each one. Over this 1000 individuals only 200 were different (these cases are those which have been effectively evaluated). In others terms, only 1,2% of possible combinations were necessary to be evaluated, that is 200 of 16384 combinations.

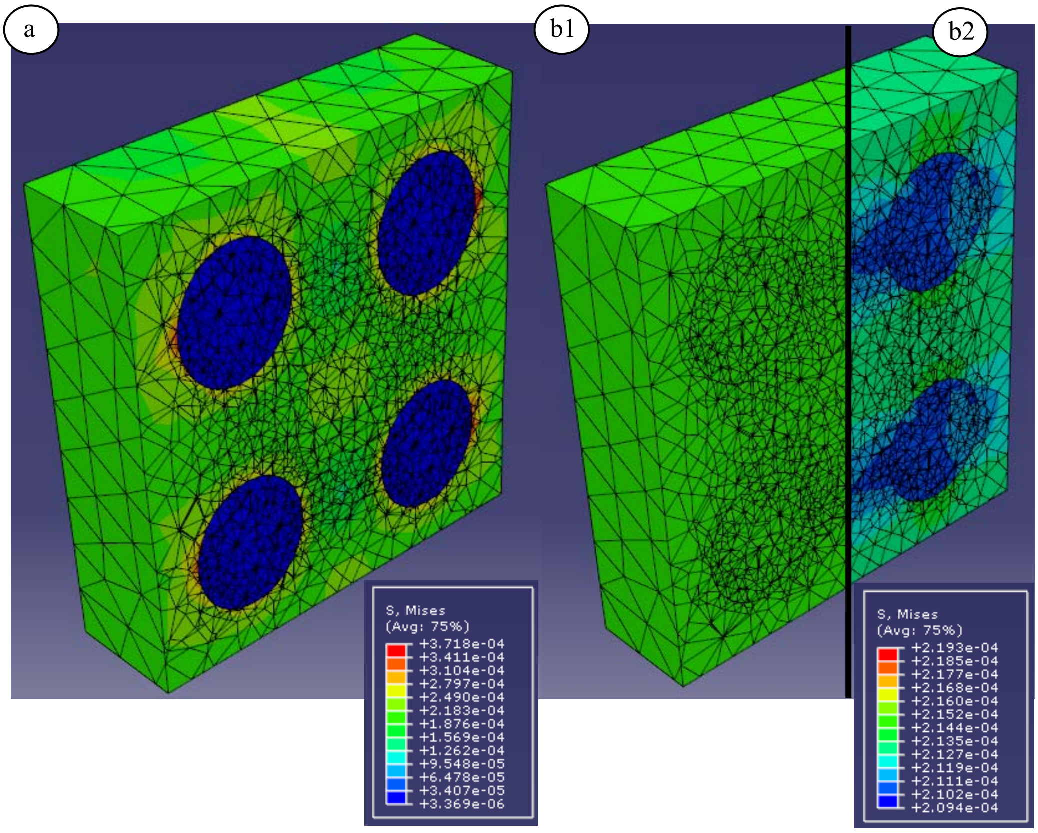

Figure 5: Distributions of Von Mises stress in the regular model with 8 spherical nodules, a) properties of the EVR study by Soares *et al.*, (2008), CV= 58,12%, b) with properties optimized to minimize the stresses, at different scale.

5. CONCLUSIONS

In the present work three optimization analyses were carried out using the GA implementation.

The studied object was a compound material built by a matrix with spherical regular in-homogeneities.

The homogeneous and linear elastic behavior is assumed for the two phases of compound.

The three cases studied are briefly described as follows:

Case A, where the determination of the in-homogeneities K and μ elastic constants, maintaining the properties of the matrix and the compound constant is proposed. Case B, where the best combination of real materials to create desired effective properties for the compound is searched, and finally Case C, where the determination of the in-homogeneities K and μ elastic parameters, keeping the properties of the matrix and the compound, trying to minimize the variation of stress in the compound is accomplished.

During the analysis of this applications, it was possible to conclude that:

- In the three studied Cases (Case A, B and C), the obtained results were the foreseeing ones, and experience was gained in different fields, that is: a) In setting the main parameters for the algorithm; b)In knowing the time to compute each individual; c) In knowing the ratio between the quantities of individuals that in each case were evaluated, and the quantity that is necessary to evaluate using the present GA implementation.

- Another important conclusion obtained is that GA procedure only approximates the optimum solution, without the need to reach it, but with an intelligent reading of the obtained results, a great information is possible to be obtained.

One of the characteristics of the GA method is not to provide the optimum value, as it was observed by several researchers, among them, Linden (2006) is cited.

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