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FINAL DEGREE PROJECT

ENGINEERING

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Study of the comparison between the
homogenization rules from classical models and
the numerical techniques (FEM)

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TABLE OF CONTENTS

1. PURPOSE AND SCOPE OF WORK.	3
2. INTRODUCTION	4
3. CLASSICAL MODELS FOR HOMOGENIZATION	5
3.1 Reuss and Voigt bounds.....	6
3.2 Hashin-Strickann upper and lower bounds	7
3.3 Eshelby method.....	9
3.4 Mori-Tanaka method.....	10
4. NUMERICAL TECHNIQUES FOR HOMOGENIZATION	12
4.1 Introduction of FEM analysis.....	12
4.2 Material Designer.....	13
4.3 Results	14
5. COMPARISON BETWEEN RESULTS FROM CLASSICAL MODELS AND FROM MATERIAL DESIGNER	16
6. CONCLUSION	18
7. LITERATURE	19
8. ACKNOWLEDGMENTS	20

1. Purpose and scope of work.

The homogenization method consists in the use of the microscopic heterogeneous material properties to calculate the effective properties of macroscopic homogeneous composite materials. To do so, there are many different technics available from literature. In this project the focus will be in:

- The Voigt and Reuss method.
- Lower and upper bounds connecting to Voigt and Reuss methods.
- Hashin-Strickann rules and its bounds.
- Eshelby method.
- Mori-Tanaka method.

Although, with the progress of the numerical approach with computational methods, such as the Finite Element Method, there are new tools to approach these problems.

An example of this kind of software is the program Ansys. This software develops, markets, and supports engineering simulation software used to predict how product designs will behave in real-world environments [1]. In this project the focus is the Material Designer tool of Ansys, that allows to calculate homogeneous composite materials and use them to test it in actual structures.

To sum up, the purpose of this work is the comparison between the classical technics of homogenization extracted from literature and the Material Designer tool.

2. Introduction

The analysis of structural behaviour of materials is topic that has developed through time, but nowadays it has taken more relevance with the need of new materials with better qualities to comply the advance of new technologies.

Traditionally, the calculations of composites were made with the classical models, in which one uses the homogenization and location techniques to provide the response of a structure, based on the properties or response of the structure's constituents [2].

Nevertheless, with the advance in numerical techniques based on computational methods, there has been created new tools to make these calculations easier and faster.

The focus of the project consists on proving the accuracy of these new techniques, specifically the tool Material Designer, in comparison with the classical techniques that engineers have been using for years.

To do so, the project begins with a description of four classical methods. For which each one is explained the hypothesis behind the model and the equations deduced by the author. Moreover, for each method there is the application of the practical problem in question on this project.

Additionally, the project shows the performance of the Material Designer software and the result of the analysis.

Finally, the project concludes with a comparison of the results and a conclusion that sums up the whole project based on the results obtained.

3. Classical models for homogenization

In this section we focus on the most common micromechanical models designated for the prediction of the effective elastic moduli of materials, in particular it is going to be proved the accuracy of these methods with the practical application in a problem of a composite with a matrix of epoxy and fibers of carbon.

Table 1 shows the properties of these materials, which later would be used in the calculations.

Material	Volume fraction	Young's Modulus X (GPa)	Young's Modulus Y (GPa)	Young's Modulus Z (GPa)
Carbon	60%	232	15	15
Epoxy	40%	5.35	5.35	5.35

Poisson's Ratio XY	Poisson's Ratio YZ	Poisson's Ratio XZ	Shear modulus XY (GPa)	Shear modulus YZ (GPa)	Shear modulus XZ (GPa)
0.279	0.49	0.279	24	5.033557	24
0.354	0.354	0.354	1.9756	1.9756	1.9756

Table 1. Carbon and Epoxy properties.

The homogenization models start with easy approximations like the Voigt and Reuss to more accurate models that estimate bounds where the value will be.

3.1 Reuss and Voigt bounds

This is the easiest model to calculate the properties of the composite material. It was developed by Voigt in 1887 and he assumed that the strain in the composite is uniform. And Reuss in 1929 believed that the stress was also uniform in the material.

With these two assumptions they developed an easy way to calculate the properties of the composite material shown in the next set of equations that they derive:

To calculate the Young's Modulus:

$$E_1 = E_{1f} * V_f + E_{1m} * V_m \quad (\text{Ec. 3.1.1})$$

$$\frac{1}{E_2} = \frac{V_f}{E_{2f}} + \frac{V_m}{E_{2m}} \quad (\text{Ec. 3.1.2})$$

For E_3 it is the same as for E_2 .

To calculate the Poisson's Ratio:

$$v_{xy} = v_{xyf} * V_f + v_{xym} * V_m \quad (\text{Ec. 3.1.3})$$

And for the other directions it is the same approximation.

Finally, to calculate the Shear modulus:

$$\frac{1}{G_1} = \frac{V_f}{G_{1f}} + \frac{V_m}{G_{1m}} \quad (\text{Ec. 3.1.4})$$

With these equations we can calculate the properties of the composite material for the practical case in this project:

Voigt and Reuss Bounds	Young's Modulus X (GPa)	Young's Modulus Y (GPa)	Young's Modulus Z (GPa)
	141.34	8.713355	8.713355

Poisson's Ratio XY	Poisson's Ratio YZ	Poisson's Ratio XZ	Shear modulus XY (GPa)	Shear modulus YZ (GPa)	Shear modulus XZ (GPa)
0.309	0.4356	0.309	4.396236493	3.108802269	4.396236493

Table 2. Voigt and Reuss bounds.

3.2 Hashin-Strickann upper and lower bounds

Hasnin and Strikman (1963) provided the strictest bounds possible from range of composite moduli for a two-phase material. They based the hypothesis on the principle of minimum potential energy and the concept of polarization. This is applied on the interaction of constituent elastic properties. This method is independent of the direction of the material data, therefore it is used for two-phase composites which the axis of isotropic material is oriented in one direction. The bounds that they developed are:

Plain strain bulk modulus

Lower bound:

$$k_l = k_2 + \frac{c_1}{1/(k_1 - k_2) + c_2/(k_2 + G_2)}$$

(Ec.3.2.1)

Upper bound:

$$k_u = k_1 + \frac{c_2}{1/(k_2 - k_1) + c_1/(k_1 + G_1)}$$

(Ec.3.2.2)

Shear modulus

Lower bound:

$$G_l = G_2 + \frac{c_1}{1/(G_1 - G_2) + c_2(k_2 + 2G_2)/2G_2(k_2 + G_2)}$$

(Ec.3.2.3)

Upper bound:

$$G_u = G_1 + \frac{c_2}{1/(G_2 - G_1) + c_1(k_1 + 2G_1)/2G_1(k_1 + G_1)}$$

(Ec.3.2.4)

Applying these equations to the properties of our practical case, it will be obtained the bounds.

First, it must be done the calculation of several parameters.

		BULK MODULUS (K)	SHEAR MODULUS (G)	PLANE STRAIN BULK MODULUS (k)
Hashin_shtrikman upper and lower bounds	Carbon	11.31	5.86	13.27
	Epoxy	6.11	1.98	6.77

Table 3. Parameters of H-S bounds.

Kl	Gl
9.7721	3.5492
ku	Gu
10.0005	3.7624

Table 4. H-S bounds

3.3 Eshelby method

The Eshelby (1957) equivalent inclusion principle uses a specific case of an ellipsoidal inclusion to the determination of elastic properties. From this it is possible to derived to other cases.

The main assumption of Eshelby's method is an infinite homogeneous matrix containing an ellipsoidal domain which is restricted by its surrounding and get from that the internal stress.

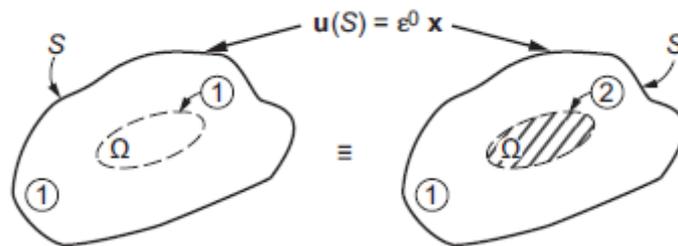


Figure 1. Eshelby method.

Through this assumptions Eshelby deduce a set of equations to calculate bulk modulus and shear modulus of a composite material.

Shear modulus:

$$\frac{\mu^*}{\mu_1} = 1 + \frac{c_2 \left(\mu_2 / \mu_1 - 1 \right)}{1 + 2 \left(\mu_2 / \mu_1 - 1 \right) P_{1212}}$$

(Ec.3.3.1)

Bulk modulus:

$$K^* = K_1 + c_2 (K_2 - K_1) (A_2)_{kkmm}$$

(Ec.3.3.2)

Eshelby tensor:

$$P_{1212} = P_{2323} = P_{1313} = \frac{4 - 5 * \nu_1}{15 * (1 - \nu_1)}$$

(Ec.3.3.3)

Strain concentration factor:

$$(A_2)_{kkmm} = \frac{4\mu_1 + 3K_1}{4\mu_1 + 3K_2}$$

(Ec.3.3.4)

Application of equations to the properties of our practical case:

P1212	Shear modulus	(A2)kkmm	Bulk modulus
0.240869163	3.578600767	1.37375724	8.452103386

Table 5. Eshelby method results of practical case.

3.4 Mori-Tanaka method

Mori and Tanaka theory's, developed in 1973, consist on the calculation of the average internal stress of a composite containing precipitates. This method used the eigenstrains, which is any mechanical deformation in a material that is not caused by an external mechanical stress.

This method assumes that the average strain of the material can be estimated by a single inclusion in an infinite matrix.

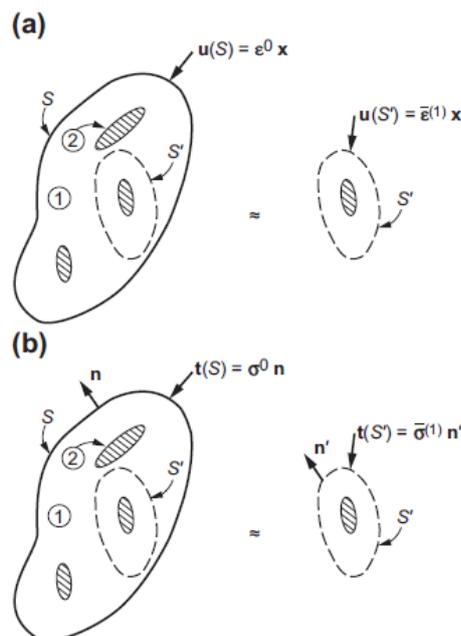


Figure 2. Mori-Tanaka method.

This hypothesis was predecessor of many papers, including the reformulation of the method by Benveniste (1987). With both theories it is possible to apply the concepts to calculate the overall bulk modulus and the effective shear modulus of a composite of two materials with different properties.

Bulk modulus:

$$K^* = K_1 + \frac{c_2(K_2 - K_1) K_1}{[(1 - c_2) (K_2 - K_1)g_1 + K_1]} \quad (\text{Ec.3.4.1})$$

$$g_1 = 3K_1/(3K_1 + 4\mu_1) \quad (\text{Ec.3.4.2})$$

Shear modulus:

$$\mu^* = \mu_1 + \frac{c_2(\mu_2 - \mu_1)\mu_1}{(1 - c_2)(\mu_2 - \mu_1)\beta_1 + \mu_1} \quad (\text{Ec.3.4.3})$$

$$\beta_1 = 6(K_1 + 2\mu_1)/[5(3K_1 + 4\mu_1)] \quad (\text{Ec.3.4.4})$$

With these equations we can calculate the properties of the composite material for the practical case in this project:

g1	BULK MODULUS	β_1	Shear modulus
0.591308368	8.824086178	0.481738326	3.939847441

Table 6. Mori-Tanaka result of practical case.

4. Numerical techniques for homogenization

There is needed new techniques to hurry the calculations nowadays, hence it is shown the huge improvement of softwares based on numerical techniques. This software has quite a lot of applications on the engineering field, from calculations of strength of structures to the approximations of the behaviour of fluids or thermomechanical problems.

In the field of materials, there are a lot of software that allows to make simulations of the behaviour of different materials in some situations. The focus of this paper is the tool Material Designer from the Ansys software.

4.1 Introduction of FEM analysis

The finite element method (FEM) is a numerical technique used to perform the analysis of different problems. The finite element method started with substantial advance in the modelling of different applications in various fields of engineering. The applications of the finite element method are only now starting to reach their potential [4] .

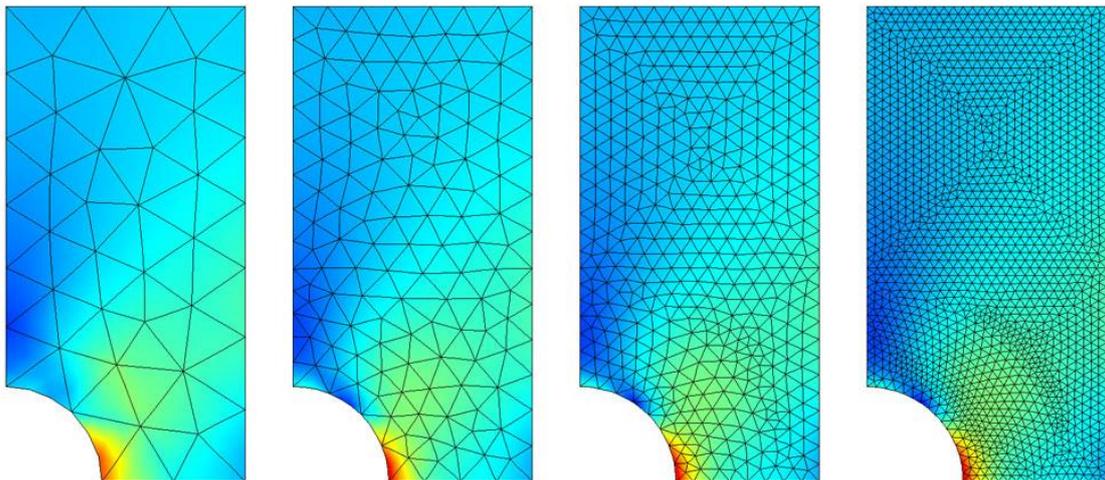


Figure 3. Different meshes.

It consists on the discretization of a problem to small elements (called mesh), where it will be considered the uniform properties, where there are

performed the calculations in a continuous element and its interpolation of equations to predict the behaviour of the whole element.

4.2 Material Designer

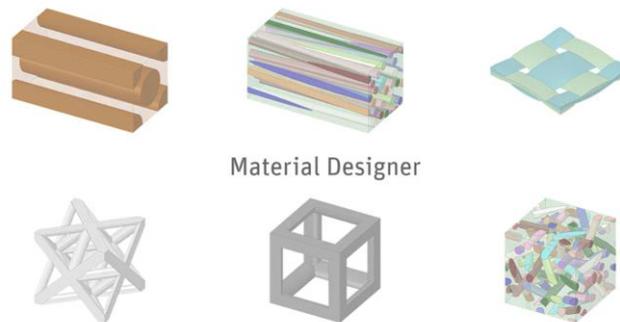


Figure 4. Material Designer.

Material designer's main use is to compute the properties of heterogeneous materials structures, for example in composites.

To do so, it defines the materials and the representative volume element (RVE) of the microstructure, which is the smallest volume over which any measurement can be taken that will give a value representative of the whole [5].

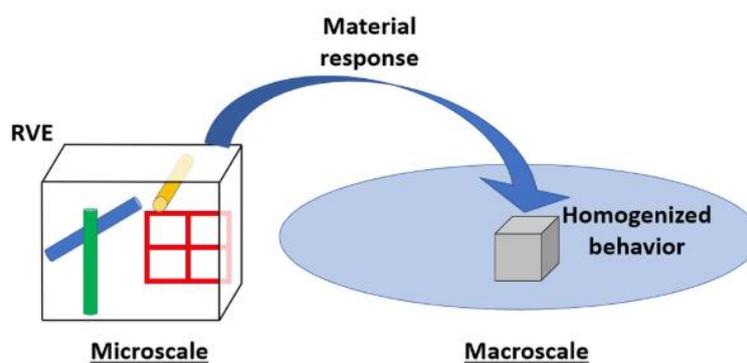


Figure 5. Transformation in Material Designer from microscale to macroscale.

Once the material is defined in volume elements the program makes the calculations and then transfer them to macroscale.

Additionally, Ansys Workbench can use the data calculated on Material Designer and use the work for other part design.

4.3 Results

The Ansys analysis of the composite has a very easy procedure, that is way is such a powerful tool, due to the simplicity and speed you can make these calculations.

It begins with the creation of the material data and the engineering data.

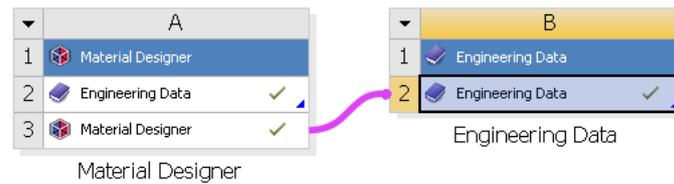


Figure 6. Material Designer in Workbench tool.

After this we add the material properties of the Carbon and the Epoxy.

	A	B	C	D	E	F	G
1	Temperature (C)	Young's Modulus X direction (Pa)	Young's Modulus Y direction (Pa)	Young's Modulus Z direction (Pa)	Poisson's Ratio XY	Poisson's Ratio YZ	Poisson's Ratio XZ
2		2,32E+11	1,5E+10	1,5E+10	0,279	0,49	0,279

Shear Modulus XY (Pa)	Shear Modulus YZ (Pa)	Shear Modulus XZ (Pa)
24	5,0336	24

Figure 7. Properties of Carbon.

Table of Properties Row 3: Isotropic Elasticity					
	A	B	C	D	E
1	Temperature (C)	Young's Modulus (Pa)	Poisson's Ratio	Bulk Modulus (Pa)	Shear Modulus (Pa)
2		5,35E+09	0,354	6,1073E+09	1,9756E+09
*					

Figure 8. Properties of Epoxy.

Once we have this, we create a geometry with a matrix of Epoxy with fibers of Carbon. The fibers have a volume fraction of 60% and a dimension of **5 μm** . Then is the formation of the mesh, that will allow the program to calculate the properties of the new material.

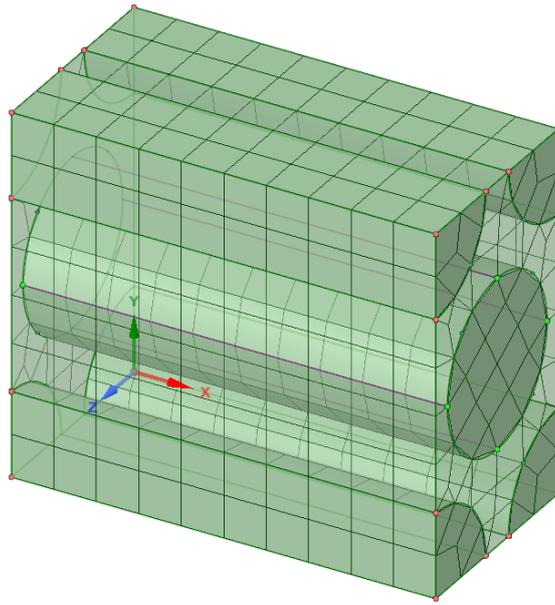


Figure 9. Mesh of new material

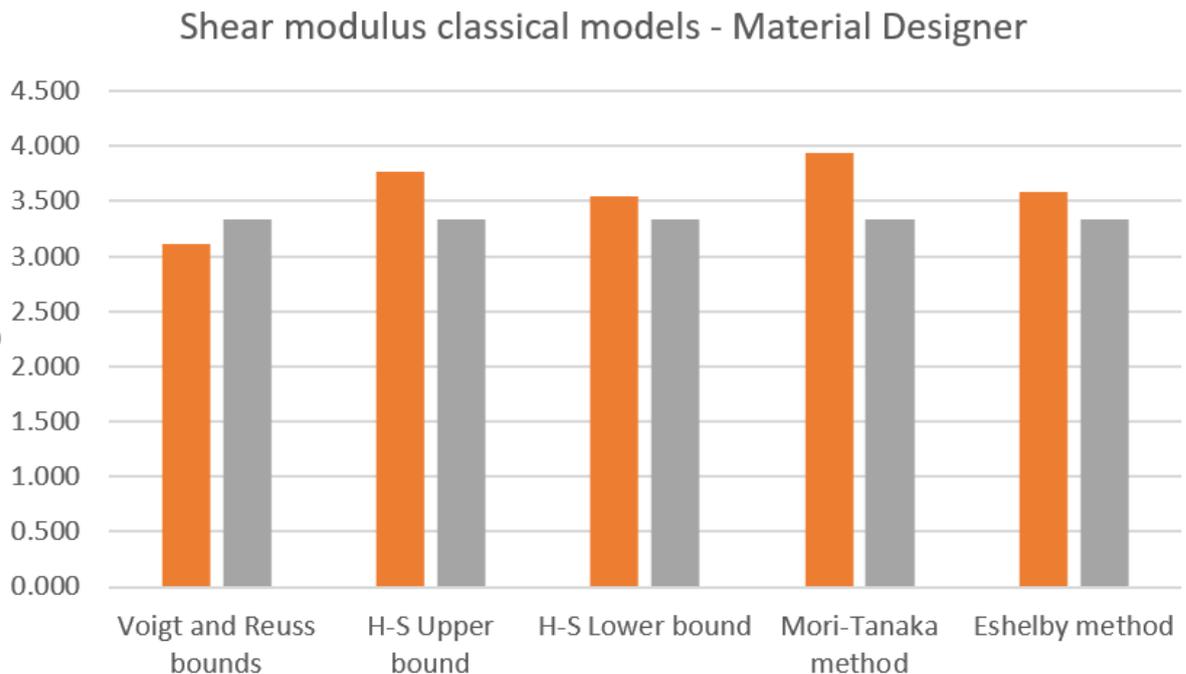
Name	Value	Unit
Engineering Constants		
E1	1,4133E+05	MPa
E2	9967,7	MPa
E3	9967,7	MPa
G12	490,85	MPa
G23	270,86	MPa
G31	490,85	MPa
nu12	0,30663	
nu13	0,30671	
nu23	0,50538	

Figure 10. Material designer results

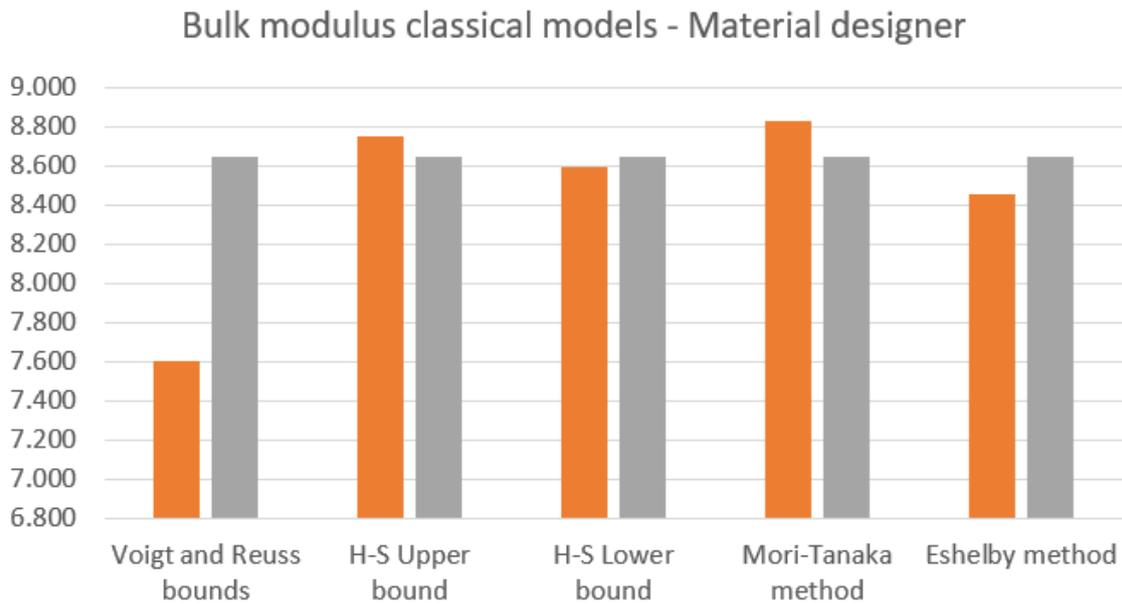
5. Comparison between results from classical models and from material designer

Comparison of results		Shear modulus		Bulk modulus	
		Classical models	Material Designer	Classical models	Material Designer
Voigt and Reuss bounds		3.11	3.34	7.60	8.64
Hashin_shtrikman upper and lower bounds	Upper	3.76	3.34	8.75	8.64
	Lower	3.55	3.34	8.59	8.64
Mori-Tanaka method		3.94	3.34	8.82	8.64
Eshelby method		3.58	3.34	8.45	8.64

Table 7. Final comparison of results.



Graphic 1. Comparison of shear modulus.



Graphic 2. Comparison of bulk modulus

The next table represents the error in the approximation between each classical method and the Material Designer results.

	Shear modulus		Bulk modulus	
	Absolut error	Relative error (%)	Absolut Error	Relative Error (%)
Voigt and Reuss bounds	0.230	6.891	1.038	12.014
H-S Upper bound	0.424	12.685	0.105	1.214
H-S Lower bound	0.210	6.299	0.052	0.606
Mori-Tanaka method	0.601	17.998	0.183	2.114
Eshelby method	0.240	7.179	0.189	2.191

Table 8. Absolute and relative error of comparison.

6. Conclusion

In conclusion, this project has shown that the Ansys tool Material Designer it is a reliable software to calculate the properties of the homogenization of two materials into one composite.

This has been shown with the comparison with different models that have been used for hundreds of years, and it is clear in the section 5 of this project that it provides an accurate solution for this problem.

7. Literature

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Link: <https://www.ansys.com/blog/how-to-simulate-microstructures-composites>

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