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OPTIMIZATION OF CONSTITUTIVE PARAMETERS FOR HYPERELASTIC MODELS SATISFYING THE BAKER-ERICKSEN INEQUALITIES

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Abstract. Hyperelastic models are used to model the mechanical behavior of rubber-like materials ranging from elastomers, such as natural rubber and silicon, to biologic materials, such as muscles and skin tissue. Once the desired hyperelastic model has its parameters fitted to the available experimental results, these hyperelastic parameters have to fulfill the requirements imposed by the Baker-Ericksen inequalities in order to guarantee a plausible physical behavior to the material. When applied to an incompressible isotropic hyperelastic model, these inequalities state that the first derivative of the strain energy density function with respect to the first strain invariant must be positive and the first derivative of the strain energy density function with respect to the second strain invariant must be non-negative. The aim of this work is to present an algorithm used to fit hyperelastic models to experimental data so that the parameters automatically fulfill the requirements of the Baker-Ericksen inequalities. This is accomplished through a constrained optimization procedure. Results obtained for natural rubber and silicon samples considering classical and newly developed hyperelastic models are shown and discussed.

1 INTRODUCTION

As the applications with rubber-like materials in the industry increased and their mechanical behavior started to be investigated more deeply, several authors have been pointing out about the necessity of imposing mathematical restrictions to the strain energy density functions of these materials, in order to guarantee their positivity, monotonicity, unicity of solutions, numerical stability and assure that the material will behave in a physically plausible way (see Truesdell, 1956; Truesdell and Noll, 1965; Bilgili, 2004; Balzani et al., 2006; Stumpf, 2009).

Truesdell and Noll (1965) have cited seven different types of conditions to be satisfied by any material so its mechanical behavior is compatible with the known laws of physics. Among these conditions is the Baker-Ericksen inequalities (Baker and Ericksen, 1954) which state that, in a compressible isotropic elastic solid body under deformation, the largest principal stress must be aligned with the largest principal strain.

According to Balzani et al. (2006) the constitutive equations written as functions of the strain energy density must satisfy general requirements of convexity, in order to assure numerical stability and a physically plausible behavior of the material. Ball (1977) introduced the convexity concept of *polyconvexity*, which was later shown by Ogden (1984) and Hartmann and Neff (2003) to automatically satisfy the Baker-Ericksen inequalities, when applied to a strain energy density function.

Truesdell and Noll (1965) concluded that when applied to incompressible isotropic materials, the Baker-Ericksen inequalities are satisfied by guaranteeing the positivity of the first derivative of the strain energy density function (W) with respect to the first strain invariant (I) and the non-negativity of the first derivative of with respect to the second train invariant (II). These conditions were analytically determined to the models analyzed in this work.

It is important to note that, in some cases, better stress-strain fittings are achieved if the Baker-Ericksen inequalities are neglected, however there is no mathematical guarantee that, outside the calibration range of strain, the material will not behave badly. When complex simulations take place, there could be particular regions in which the material experiments strains higher than those for which its parameters were calibrated, and in these cases it is very important to assure that, at least, its mechanical behavior do not violate any law of physics.

The aim of this paper is to apply the Baker-Ericksen inequalities to the equations of five distinct hyperelastic models, write a routine to obtain their sets of constitutive parameters that satisfy the inequalities, and then fit these models against three different sets of experimental data (simple tension, biaxial tension and pure shear) from two different elastomers samples (Treloar set of data (Jones and Treloar, 1975) and unfilled silicone rubber (Meunier et al., 2008)). An optimizing technique proposed by Stumpf (2009) that uses data from one or more sets of experimental tests simultaneously (multi-criteria optimization) and obtains the optimum constitutive parameters that minimize the error between experimental and theoretical results is used.

2 CONSTITUTIVE PARAMETERS OPTIMIZATION TECHNIQUE

In order to guarantee good results when analyzing rubber-like materials, the analyst must assure that the available experimental data to be fitted to a model represent the major type of deformation of the analyzed component. For a few simple cases, that should not represent a problem, but when a component is subjected to complex deformation, the best solution would be to calibrate the hyperelastic model to the data from more than one experimental test.

It was shown by Hoss (2009) and Stumpf (2009) that predicting the behavior of an elastomer in a deformation mode different than the one used in the fitting can lead to seriously inaccurate results. Depending on the hyperelastic model, sometimes the predictions do not even show a physically plausible behavior (Hoss, 2009), and many times leads to numerical problems when used in a finite element software.

In order to overcome this problem, Stumpf (2009) presented a methodology for fitting hyperelastic models to more than one set of experimental data simultaneously. The methodology allows the use of any combination of two or more different stress-strain tests (usually simple tension, biaxial tension, pure shear, simple shear and compression tests) and any hyperelastic model as well.

First it is necessary to know the analytical relationship between stress and strain for simple cases of deformation (homogeneous deformation). These relationships depend uniquely on the equation of the hyperelastic model and the deformation itself and Figures 1, 2 and 3 along with Equations (1), (2) and (3) show them for the three cases used in this work (in Eqs.(1-3) λ is the stretch):

$$\sigma_1 = t_T = 2\left(\lambda - \frac{1}{\lambda^2}\right)\left(\frac{\partial W}{\partial I} + \frac{1}{\lambda}\frac{\partial W}{\partial II}\right) \tag{1}$$

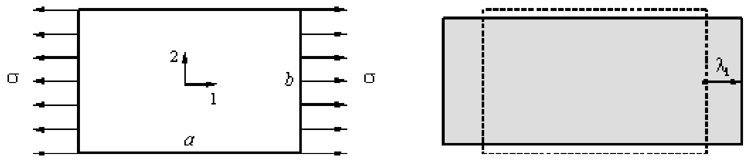


Figure 1: Simple tension case of deformation - Eq.(1)

$$\sigma_1 = \sigma_2 = t_B = 2\left(\lambda - \frac{1}{\lambda^5}\right)\left(\frac{\partial W}{\partial I} + \lambda^2\frac{\partial W}{\partial II}\right) \tag{2}$$

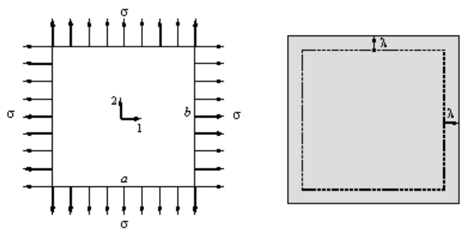


Figure 2: Biaxial tension case of deformation - Eq.(2)

$$\sigma_1 = t_P = 2\left(\lambda - \frac{1}{\lambda^3}\right)\left(\frac{\partial W}{\partial I} + \frac{\partial W}{\partial II}\right) \tag{3}$$

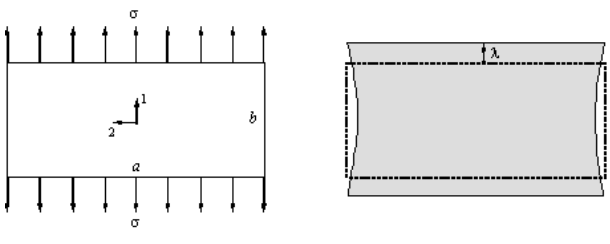


Figure 3: Pure shear case of deformation - Eq.(3)

Using the experimental values of strains (or stretches, since $\lambda = \varepsilon + 1$, where ε is the true deformation) and the derivatives of the strain energy density functions in the above equations, each one will represent the theoretical stress for every experimental point, in terms of the constitutive coefficients of each particular model, for each deformation case. Figure 4 shows examples of differences usually obtained between experimental and theoretical results for the three cases of deformation used in this work.

By subtracting the theoretical stresses the experimental values of stress due to each test, squaring this difference and summing between the desired distinct deformation cases, we obtain the error function to be minimized, given by:

$$E = e_T + e_P + e_B = \sum_{i=1}^{n_T} \left(t_{T_i} - t_{E_i}\right)_T^2 + \sum_{j=1}^{n_P} \left(t_{T_j} - t_{E_j}\right)_P^2 + \sum_{k=1}^{n_B} \left(t_{T_k} - t_{E_k}\right)_B^2 \tag{4}$$

where n_T, n_P and n_B are the number of points in available single tension, pure shear and biaxial tension experimental data respectively, t_T and t_E are the theoretical and experimental values for the stresses respectively and the sub indexes T, B and P refer to single tension, biaxial tension and pure shear tests respectively.

The problem lies now in obtaining the constitutive coefficients that minimize the error function E:

$$\min_{\mathbf{C}} E(\mathbf{C}) \tag{5}$$

where $E(C)$ is the error function in terms of the set of constitutive coefficients C.

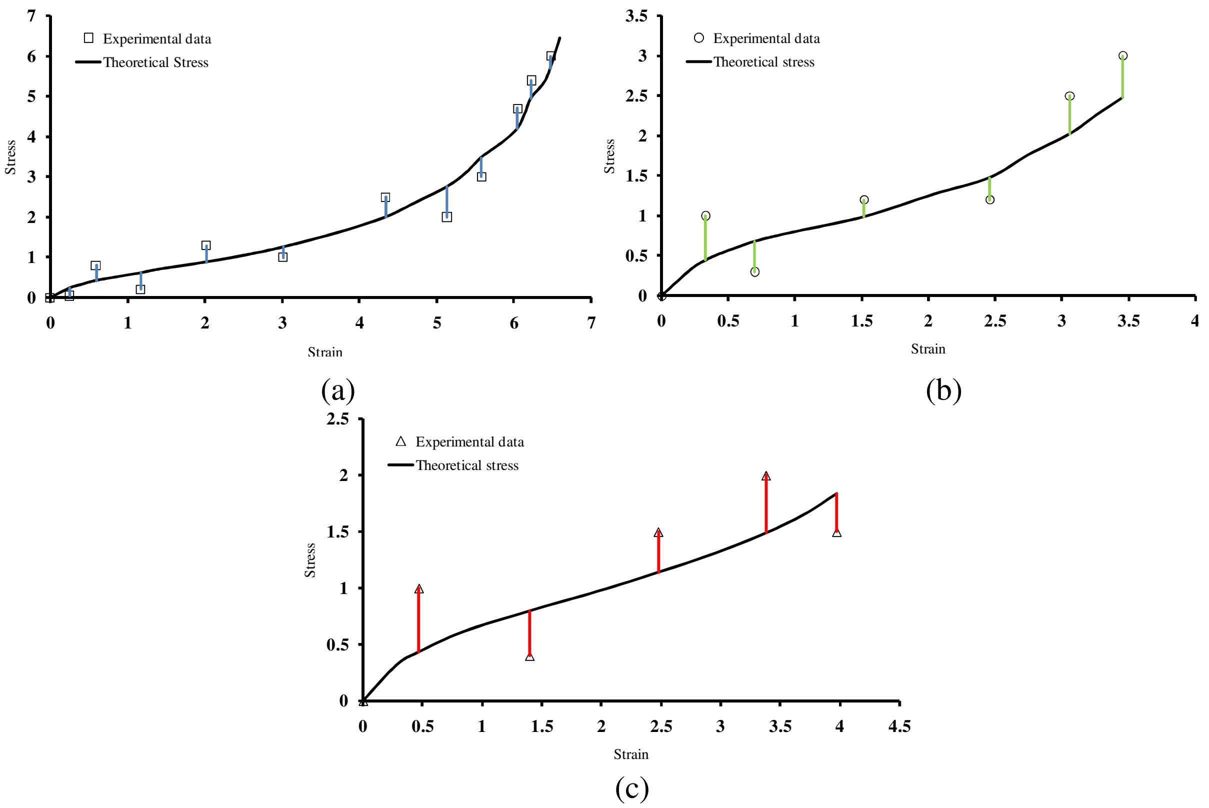


Figure 4: Gaps between experimental and theoretical results obtained for (a) simple tension deformation, (b) biaxial tension deformation and (c) pure shear deformation

This methodology consists in an optimization technique, since it obtains the optimum set of coefficients for any hyperelastic model that will lead to the minimum error between experimental and theoretical results for two or more distinct sets of data simultaneously.

Compared to the classical methodology in which, for each different deformation case, an exclusive set of coefficients is obtained, the optimization methodology proposed present great advantage, since one single set of constants are used for any deformation case, or combination of them.

If no restrictions are imposed to the set of constants C, this can be solved as a problem of optimization without restrictions, but in this paper, due to the conditions imposed by the Baker-Ericksen inequalities, it had to be evaluated as a problem of optimization with restrictions. Matlab's routine *fmincon* was used in the present work (Matlab, 2008).

3 APPLYING THE INEQUALITIES TO THE MODELS

In order to apply the Baker-Ericksen inequalities to the hyperelastic models, it is first necessary to obtain their first derivatives with respect to the first and second strain invariants. After that, the conditions to be satisfied by the parameters of each model are analytically developed and inserted into the Matlab routine.

The following models and their respective restrictions were analyzed in this paper:

- HMLSI (Hoss, 2009):

$$W = \frac{\alpha}{\beta}\left(1 - e^{-\beta(I-3)}\right) + \frac{\mu}{2b}\left[\left(1 + \frac{b(I-3)}{n}\right)^{n} - 1\right] \tag{6}$$

$$\frac{\partial W}{\partial I} = \alpha e^{-\beta(I-3)} + \frac{\mu}{2}\left(1 + \frac{b(I-3)}{n}\right)^{n-1} > 0 \tag{7}$$

$$\frac{\partial W}{\partial II} = 0 \tag{8}$$

where α, β, μ, b and n are fitting constitutive parameters and I is the first strain invariant.

As seen in the inequality of the Equation (7), it is not possible just by inspection to determine analytically the restrictions to be applied to the parameters of the HMLSI model. This inequality has to be checked at each point of the deformation range, so it was developed a brief code in Maple (Maple, 2003) to check it along the stress-strain data.

- HMHSI (Hoss, 2009):

$$W = \frac{\alpha}{\beta}\left(1 - e^{-\beta(I-3)}\right) + \frac{\mu}{2b}\left[\left(1 + \frac{b(I-3)}{n}\right)^{n} - 1\right] + C_2 \ln\left(\frac{II}{3}\right) \tag{9}$$

$$\frac{\partial W}{\partial I} = \alpha e^{-\beta(I-3)} + \frac{\mu}{2}\left(1 + \frac{b(I-3)}{n}\right)^{n-1} > 0 \tag{10}$$

$$\frac{\partial W}{\partial II} = \frac{C_2}{II} \geq 0 \tag{11}$$

where C_2 is a fitting parameter and II is the second strain invariant.

The first derivative in Equation (10) is the same as for the HMLSI model in Equation (7), so the same approach was used to check this model´s parameters. Equation (11) however, tells us the restriction to the parameter C_2:

$$C_2 \geq 0 \tag{12}$$

- 3-terms Yeoh (Yeoh, 1990):

$$W = C_1(I-3) + C_2(I-3)^2 + C_3(I-3)^3 \tag{13}$$

where I is the first strain invariant, II is the second strain invariant and C_1, C_2 and C_3 are fitting constitutive parameters.

Its derivatives with respect to the first and second strain invariants are, respectively:

$$\frac{\partial W}{\partial I} = C_1 + 2C_2(I-3) + 3C_3(I-3)^2 > 0 \tag{14}$$

$$\frac{\partial W}{\partial II} = 0 \geq 0 \tag{15}$$

Although Equation (15) is not the only possible condition to satisfy the Baker-Ericksen inequalities in this case, it was chosen to guarantee the positivity of the parameters C_1, C_2 and C_3 in the Yeoh model.

Thus, for the Yeoh model, in order to assure the satisfaction of the Baker-Ericksen inequalities, the conditions its parameters have to fulfill are:

$$\begin{aligned} C_1 &> 0 \\ C_2 &> 0 \\ C_3 &> 0 \end{aligned} \tag{16}$$

- Fung (Fung, 1967):

$$W = \frac{\mu}{2b}\left(e^{b(I-3)} - 1\right) \tag{17}$$

where μ and b are fitting constitutive parameters.

The first derivative with respect to the strain invariant is:

$$\frac{\partial W}{\partial I} = \frac{\mu}{2} e^{b(I-3)} > 0 \tag{18}$$

The term $(I-3)$, if any deformation occurs in the components, is always positive, and so the exponential term $e^{b(I-3)}$. Thus, for the Fung model, the only condition necessary to satisfy the Baker-Ericksen inequalities is:

$$\mu > 0 \tag{19}$$

- Pucci-Saccomandi (Pucci and Saccomandi, 2002):

$$W = -\frac{\mu\, J_L}{2} \ln\left(1 - \frac{I-3}{J_L}\right) + C_2 \ln\left(\frac{II}{3}\right) \tag{20}$$

where C_2, μ and J_L are fitting constitutive parameters.

Equation (21) shows the first derivative of the Pucci-Saccomandi model with respect to the first strain invariant:

$$\frac{\partial W}{\partial I} = \frac{\mu}{2\left(1 - \dfrac{I-3}{J_L}\right)} > 0 \tag{21}$$

An initial condition inherent to the model is that the parameter J_L should always be higher than the term $(I-3)$. The term between parentheses in the denominator is, then, always positive. This leads to the condition:

$$\mu > 0 \tag{22}$$

The derivative of W with respect to the second strain invariant leads to the second condition for the Pucci-Saccomandi model:

$$C_2 \geq 0 \tag{23}$$

For each model analyzed two Matlab codes were written: one concerning the analytical equation for the error to be minimized as presented in the optimization methodology of Section 1 and another containing the restrictions imposed by the Baker-Ericksen inequalities as detailed in this section. These two routines are sufficient for the Matlab command *fmincon* to perform the optimization.

4 THE EXPERIMENTAL DATA

The experimental data used in this paper were due to simple tension (T), biaxial tension (B) and pure shear (P) tests in samples of:

- Treloar set of data (Treloar);
- Unfilled silicone rubber (USR).

Figures 5 and 6 show the stress-strain relation for these three cases of deformation for each elastomer sample:

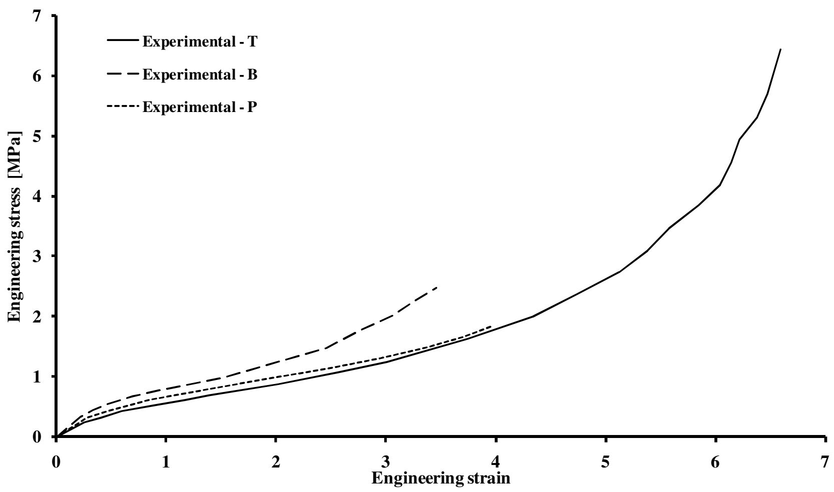


Figure 5: Set of Treloar experimental data.

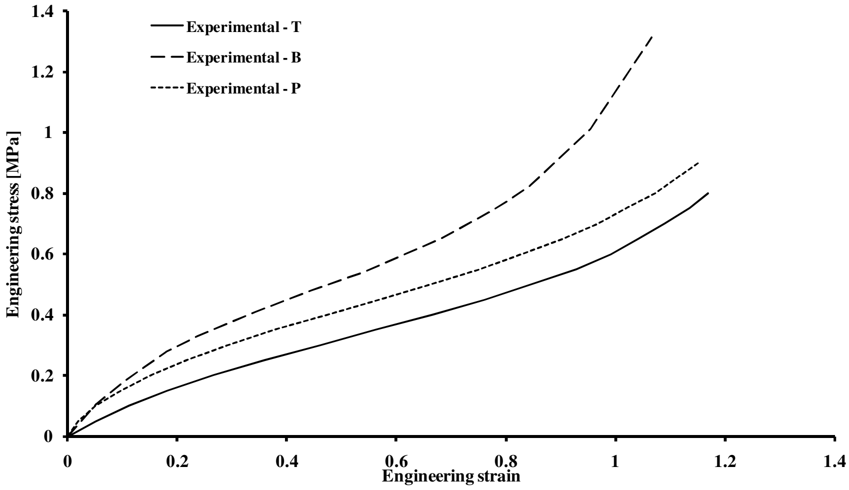
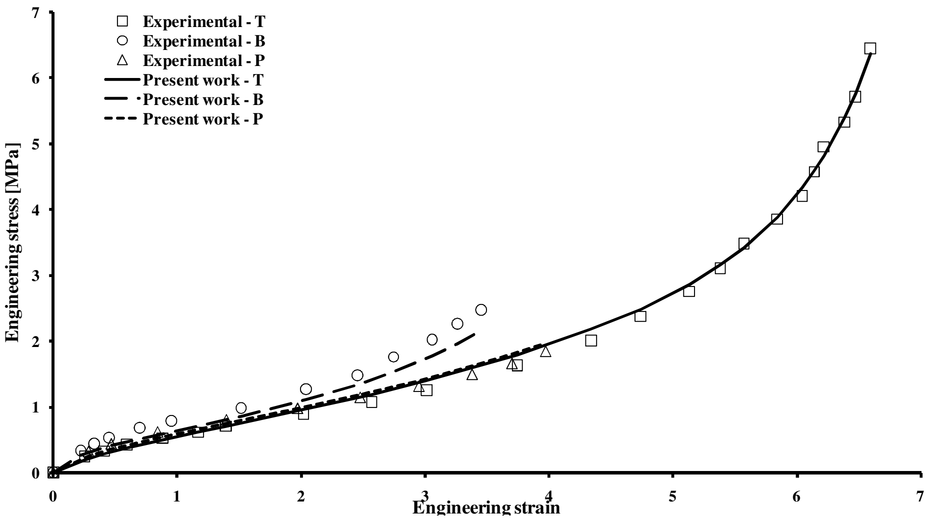


Figure 6: Experimental data for the USR samples

5 RESULTS

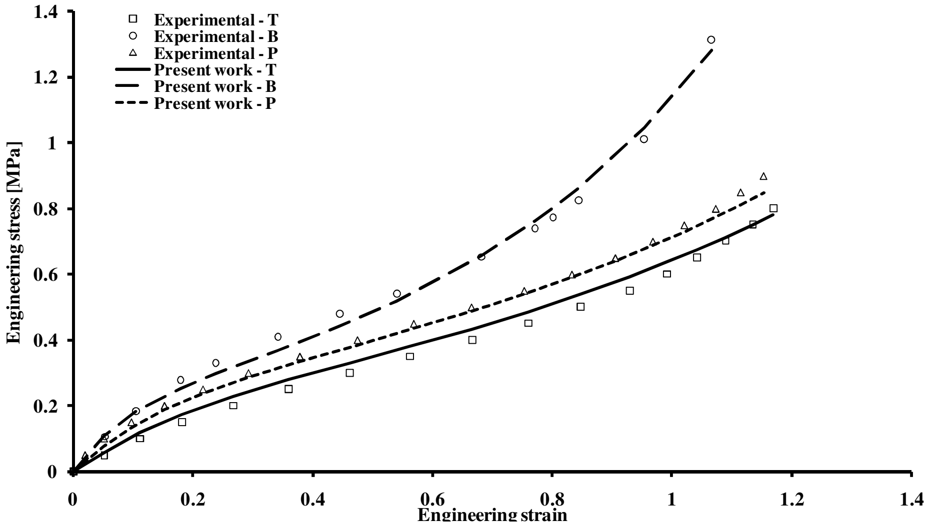
The results obtained when the methodology was applied for the HMLSI model to the Treloar and USR data are shown in Figures 7 and 8 respectively, along with the constitutive coefficients obtained in each case. The sets of coefficients showed in each of the Figures 7 to 16 satisfy their respective inequalities determined in Equations (7), (12), (16), (19), (22) and (23).

It is observed very good agreement between experimental and theoretical data for the three different types of deformation and for all samples. The coefficients presented in each figure, in addition to be those that minimize the error of Equation (4), also satisfy the Baker-Ericksen inequality of Equation (7).



α	0.153
β	-0.0106
b	0.166
n	24.8
μ	1.73E-4

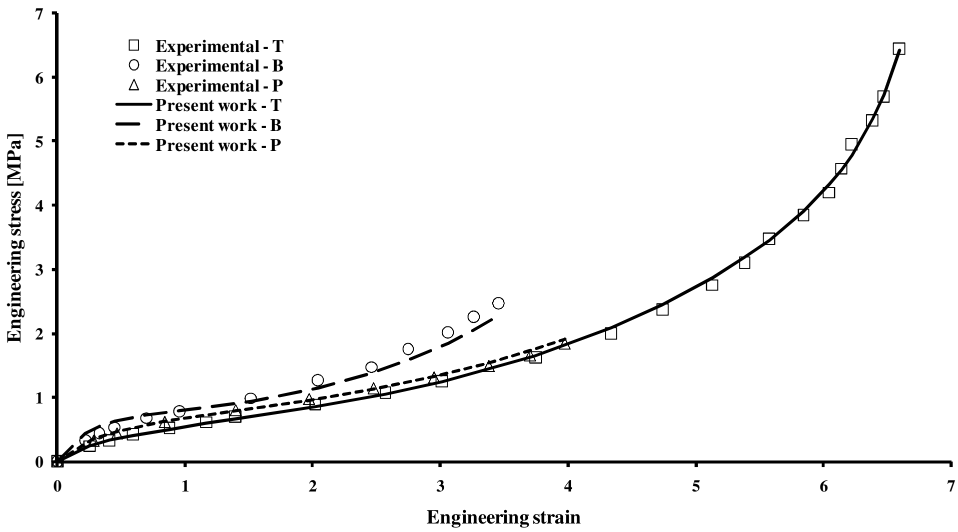
Figure 7: Optimized set of coefficients - Treloar set of experimental data and HMLSI model



α	0.12
β	-0.167
b	1.03
n	0.25
μ	0.166

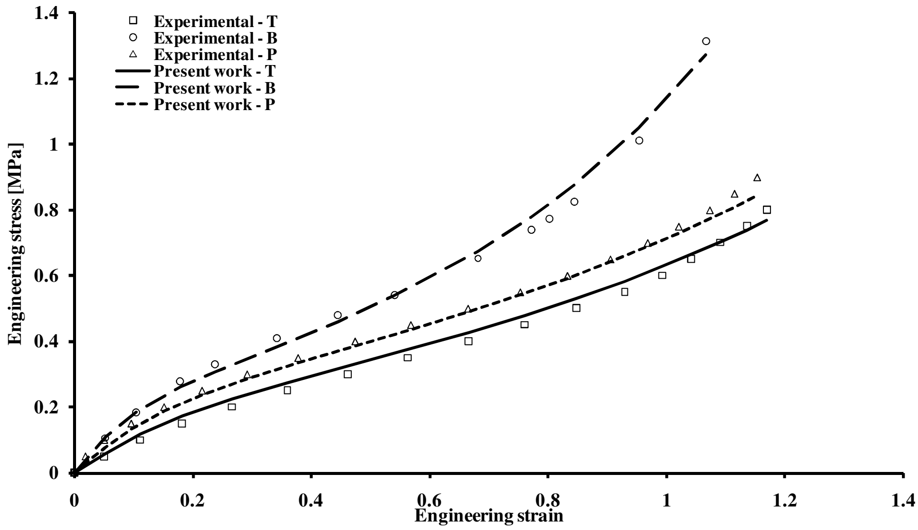
Figure 8: Optimized set of coefficients - USR set of experimental data and HMLSI model

For the HMHSI model, Figures 9 and 10 show analog results to those above:



α	0.112
β	-0.0208
b	31.2
n	14.7
μ	0
C_2	0.337

Figure 9: Optimized set of coefficients - Treloar set of experimental data and HMHSI model

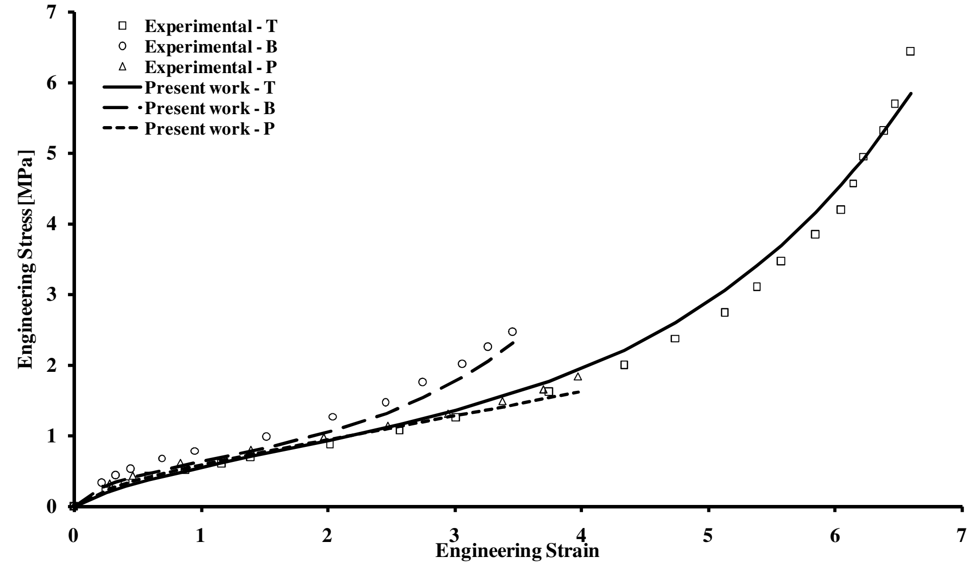


α	0.121
β	-0.161
b	0.537
n	0.112
μ	0.142
C_2	0.0407

Figure 10: Optimized set of coefficients - USR set of experimental data and HMHSI model

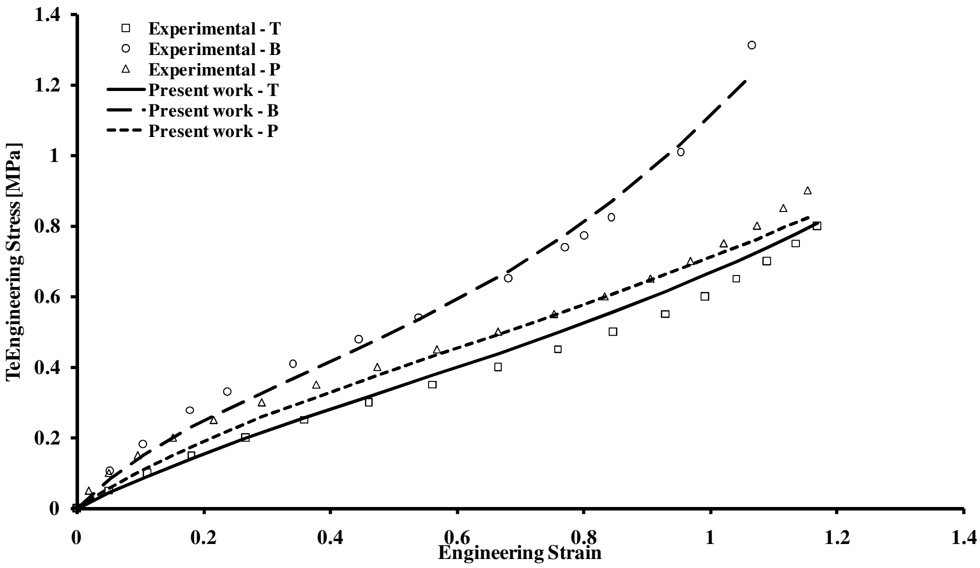
Like the HMLSI model, the HMHSI model showed very good agreement between practical and theoretical results.

Results for the 3-terms Yeoh model are presented in Figures 11 and 12 for the simple tension, biaxial tension and pure shear test for the Treloar and USR samples.



C_1	0.159
C_2	0
C_3	2.51E-5

Figure 11: Optimized set of coefficients - Treloar set of experimental data and 3-terms Yeoh model

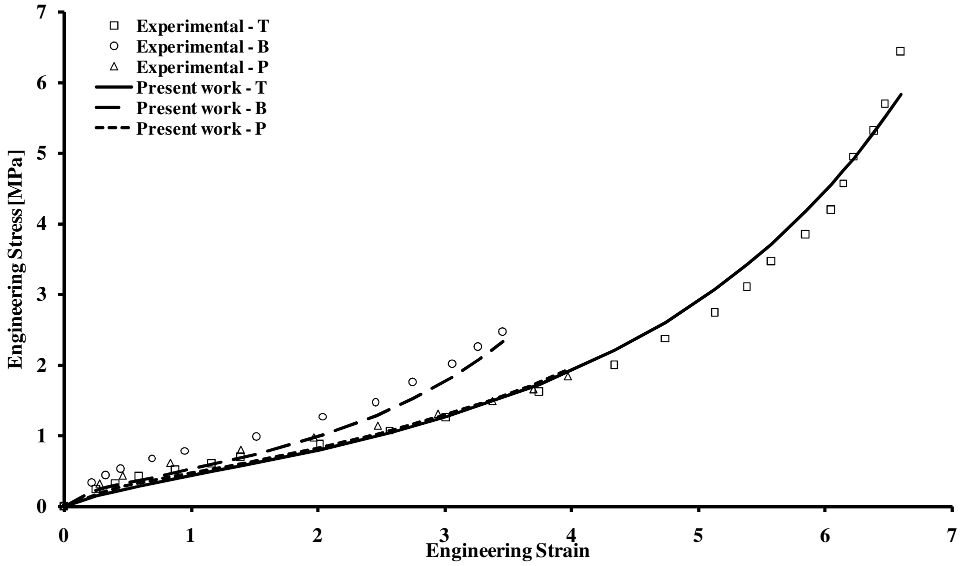


C_1	0.152
C_2	7.83E-3
C_3	6.73E-4

Figure 12: Optimized set of coefficients - USR set of experimental data and 3-terms Yeoh model

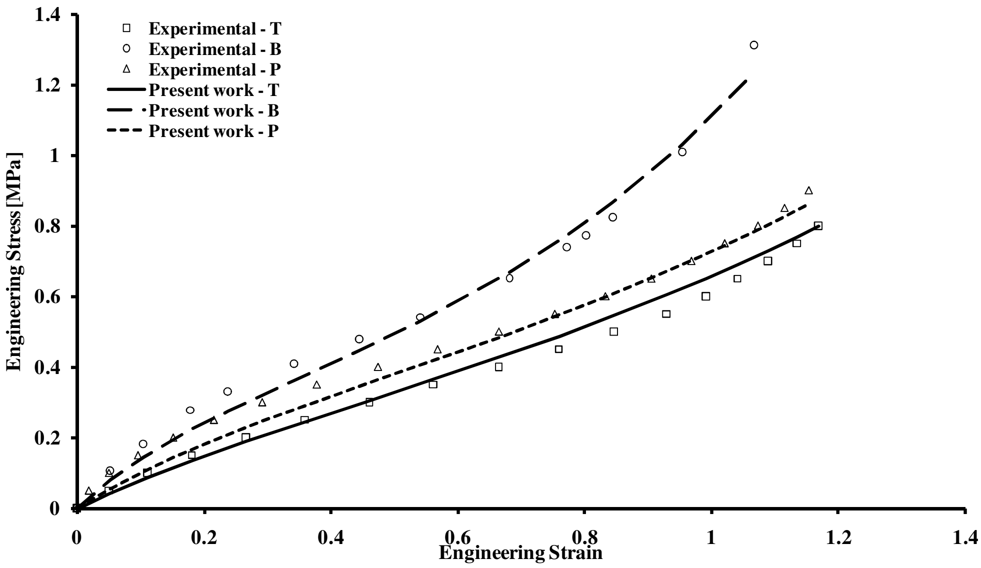
It is observed again, for the two cases, good agreement between experimental and theoretical results.

When applied to the Fung model, the methodology had also led to similarly good quantitative and qualitative results. They are shown in Figures 13 and 14.



μ	0.24
b	0.0212

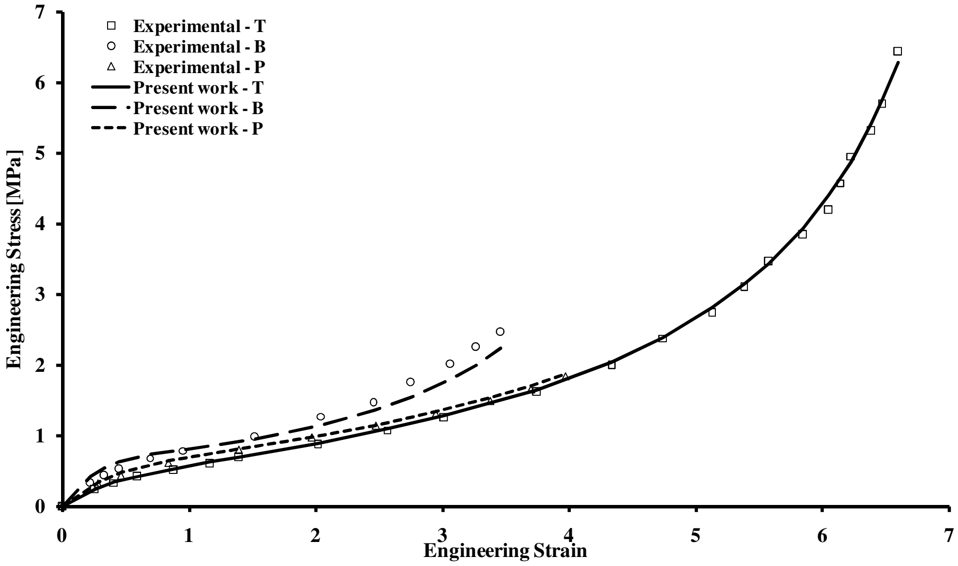
Figure 13: Optimized set of coefficients - Treloar set of experimental data fitted and Fung model



μ	0.2889
b	0.132

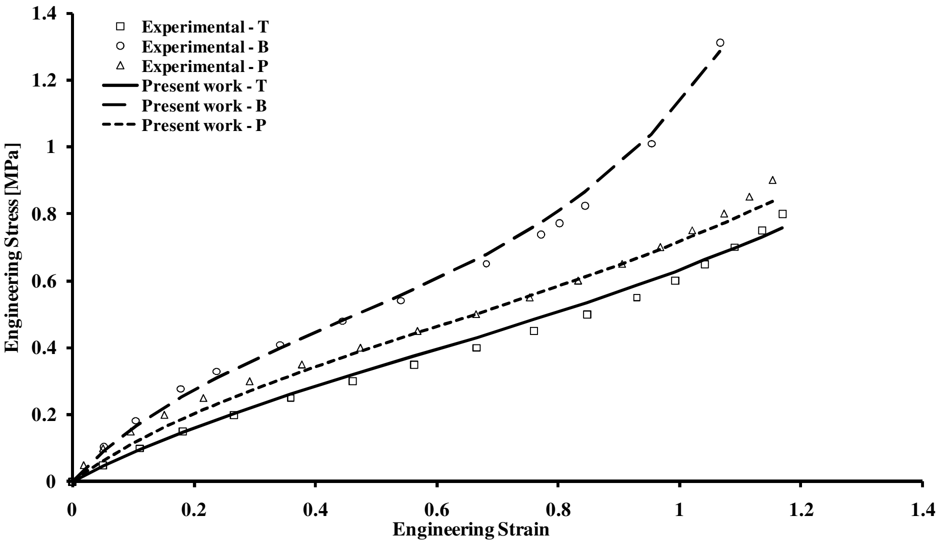
Figure 14: Optimized set of coefficients - USR set of experimental data and Fung model

Figures 15 and 16 show analog results when analyzing the Pucci-Saccomandi model.



μ	0.254
J_L	82.3
C_2	0.294

Figure 15: Optimized set of coefficients - Treloar set of experimental data and Pucci-Saccomandi model



μ	0.282
J_L	13.5
C_2	0.0621

Figure 16: Optimized set of coefficients - USR set of experimental data and Pucci-Saccomandi model

All the graphics in the Figures 7 to 16 were plotted using the optimized coefficients listed aside each one. These coefficients assure, for each model and each set of experimental data, the physically plausible behavior of these materials not only along the ranges of strain analyzed, but for any possible strain level.

For the sake of comparison of the classical prediction methodology - in which the model is fitted for a single case of deformation and the obtained constants are used to *predict* its behavior under a distinct case of deformation - and the optimization methodology presented in Section 2, they were applied to the HMLSI model and the USR set of experimental data.

First, using the classical least square technique, the HMLSI model was calibrated against the data for single tension of the USR sample. The parameters obtained were used to *predict* the model behavior under the *other two cases of deformation*: biaxial tension and pure shear. Second, the model was fitted against the data for biaxial tension of the USR sample and those constants were used to *predict* its behavior under single tension and pure shear. Last, the model was fitted against pure shear data and its *predicted* behavior under single tension and biaxial tension was analyzed.

The intention is to show that, even if a model fits accurately with a single set of experimental data, caution should be taken when using these parameters to simulate the elastomer behavior under a different, or even a combined, case of deformation.

What one can see in Figures 17, 18 and 19 is the comparison between prediction results. Figure 17 show the *predictive behaviors* for single tension deformation of USR sample, when the HMLSI model was fitted against biaxial tension, pure shear and the methodology proposed in this work.

Figure 18 shows the *predictive behaviors* for biaxial tension of USR sample when the HMLSI model is fitted for the single tension, pure shear data and the methodology proposed.

Last, Figure 19 shows a comparison of the *predictive behaviors* for USR sample under pure shear deformation when it is fitted against single tension, biaxial tension data and when applied the proposed method, again for the HMLSI model.

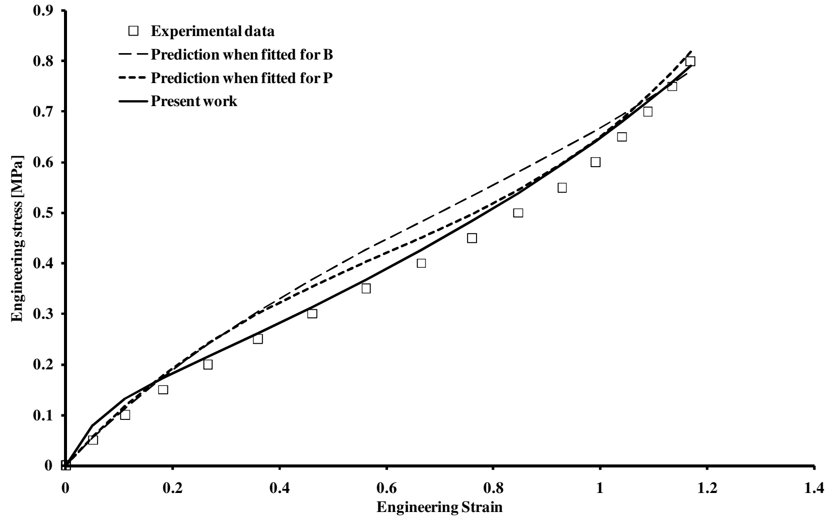


Figure 17: Prediction of the behavior of USR samples under simple tension case of deformation when the constants of the HMLSI model are fitted against biaxial tension, pure shear data and the method presented

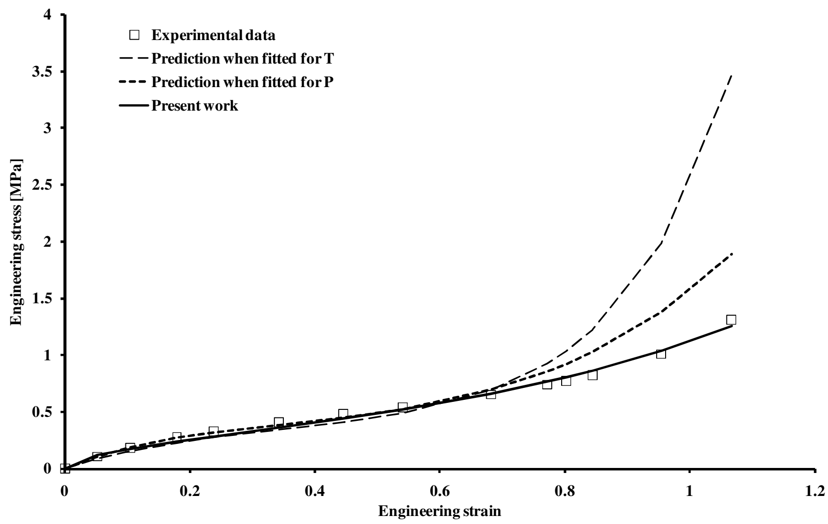


Figure 18: Prediction of the behavior of USR samples under biaxial tension case of deformation when the constants of the HMLSI model are fitted against single tension, pure shear data and the method presented

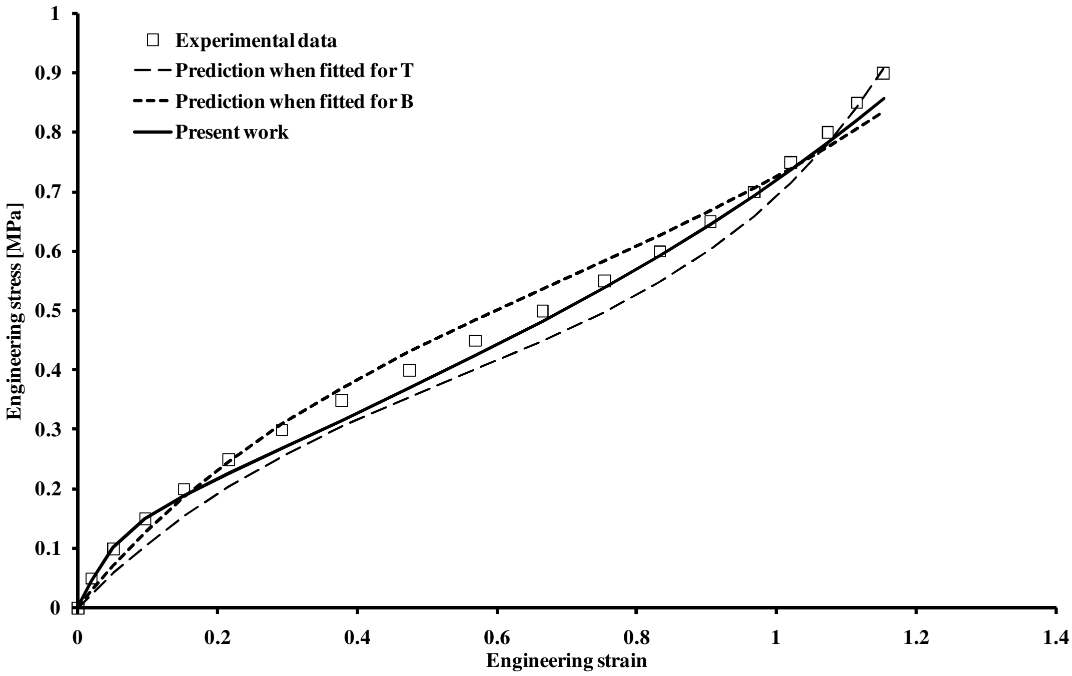


Figure 19: Prediction of the behavior of USR samples under biaxial tension case of deformation when the constants of the HMLSI model are fitted against single tension and pure shear data and the method presented

For the three cases, the optimization methodology proposed in Equations (4) and (5) presented better results than the predictive ones. It should be pointed out that for each graphic in Figures 17, 18 and 19, there is a different set of constants when applying the classical least square technique, whereas for the proposed methodology, a single set of constants is used to plot those three graphics.

6 CONCLUSIONS

This paper presented a methodology to obtain constitutive parameters of hyperelastic materials throughout a restricted optimization technique. The restrictions imposed to the parameters were derived analytically after applying the Baker-Ericksen inequalities to each model. In three out of five models, analytical restrictions were obtained, but for the HMLSI and HMHSI models, it was necessary to check them along the strain range in each point through a separate Maple routine.

The optimization technique was based in the work of Stumpf (2009) which uses experimental data originated from two or more distinct cases of deformation simultaneously. Therefore an optimum set of constitutive coefficients is obtained in such a way that it minimizes error between experimental and theoretical results for all deformation modes considered. In this paper, that methodology was extended by adding restrictions to the algorithm and solving the problem using a Matlab optimization routine called *fmincon*.

Experimental data due to three different deformation cases (simple tension, biaxial tension and pure shear) and two different elastomers samples (Treloar set of data and unfilled silicone rubber) were used to calibrate five different hyperelastic models (HMLSI, HMHSI, 3-terms Yeoh, Fung and Pucci-Saccomandi) and the results were presented in Section 5. In all cases, the sets of coefficients satisfied the restrictions imposed by the Baker-Ericksen inequalities.

As one can conclude from Figures 7 to 16, theoretical results fitted the experimental data of the three cases of deformation accurately in all cases, which is very unlikely to observe when a model is calibrated for a single deformation case and its fitted parameters are used to predict the elastomer´s behavior for a distinct case, as demonstrated in the final part of Section 5.

Moreover, these coefficients also satisfy the Baker-Ericksen inequalities, which guarantees that, for all ranges of strain - and not only for that the model was fitted to - these materials will behave in a physically plausible way.

The methodology is also characterized by its flexibility, since through modification of Equation (4) by including or eliminating the desired terms, the user can suit the method to the available experimental data, making it capable to be used to any combination of deformation cases and any hyperelastic model.

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