The implications of constitutive model selection in hyperelastic parameter identification

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ABSTRACT: Hyperelastic constitutive models are investigated and compared on their ability to predict the elastic, isothermal and rate-independent response of rubber. Constitutive model parameters are identified in an optimization problem by minimizing the difference between homogeneous experimental data and their analytical solutions. The results are presented for ten hyperelastic constitutive models over four case studies where varying extents of experimental data are used. The choice of constitutive model is found to determine how accurately experimental data is fitted, though this has different implications depending on the extent of available experimental data. With a complete data set, an accurate fit generally indicates an overall accurate prediction of the material's response. However, an accurate fit to a reduced set of experimental data may not indicate an accurate prediction of the overall response. With reduced data, accurate predictions are obtained only if the constitutive model is capable of predicting unfitted deformations and the appropriate experimental data is used.

1 INTRODUCTION

Hyperelastic constitutive models are used in the prediction of the elastic, isothermal and rate-independent behavior of rubber, and similar materials. When more complex behavior is considered, such as time-dependence or inelasticity, a hyperelastic constitutive model may be used as the ground-state elastic response, shown to be experimentally valid by Miehe and Keck (2000). In either case, it is of importance to identify the parameters of the hyperelastic constitutive model by way of physical experiments on the material of interest. The aim of this study is to investigate how the choice of hyperelastic constitutive model affects the outcome of parameter identification methods.

The nonlinear stress response of rubber is dependent on both the strain magnitude and its applied mode of deformation. To ensure that the identification of hyperelastic parameters is comprehensive, a depth of experimental data is therefore desirable. For an incompressible material, an assumption often applied to rubber, the complete range of possible deformations may be fully defined on an invariant plane (a plot of the first and second strain invariants I_1 and I_2. For a hyperelastic experimental data set to be considered as complete, the experiments should cover a strain range that encapsulates the deformations expected by the component of interest.

An example of a complete set of experiments is that from Treloar (1944). This data consists of uniaxial tension (UT) and equibiaxial tension (ET) experiments, which form the outer bounds of the possible deformations of the invariant plane, as well as pure shear (PS) data from a planar tension test, for which I_1 and I_2 are equal. Alternatively, general biaxial data can fully traverse the invariant plane and is also considered as complete data, as used by Jones and Treloar (1975) and Kawabata et al. (1981). The primary advantage of both of these complete data sets is their use of so-called homogeneous experiments. With the assumption of homogeneity, low computational cost analytical solutions for these deformations may be derived for most constitutive models. This enables a wide range of optimization methods to identify constitutive model parameters in a minimization problem.

It is assumed here that an accurate fit to a complete set of experimental data implies that predictions of the material will be similarly accurate, within the experimented strain range. In this case the chosen constitutive model should be that which can most accurately fit the complete data set. Studies of this nature are often used in the proposal of new hyperelastic constitutive models or in comparison studies. In the comparison study by Marckmann and Verron (2006), twenty constitutive models are ranked on their ability to fit the data of Treloar (1944) and Kawabata et al. (1981), with added credit for models with a low number of parameters and parameters that are physically defined.

The requirement of bespoke testing equipment means that gaining a complete set of experimental data may not always be a feasible option. Parameter identification with a reduced experimental data set is therefore common. It is of interest to investigate how the choice of constitutive model influences hyperelastic parameter identification when only a reduced experimental data set is available. This has been studied in part by Seibert and Schöche (2000) using uniaxial data only to predict the biaxial response and by Steinmann et al. (2012) and Hossain and Steinmann (2013) using each experiment from Treloar (1944) individually and predicting the two unfitted deformation modes. While these studies each conclusively show that the prediction of unfitted deformation modes is dependent on the choice of constitutive model, a comparison of the various models, as in Marckmann and Verron (2006), is not offered.

The present study further investigates how different constitutive models affect the outcome of parameter identification by using varying extents of experimental data. The investigation is separated into four case studies. In all case studies, the parameters of the chosen constitutive models are identified by optimization using the analytical solutions for the homogeneous experiments. In the first case study, a complete homogeneous data set is used, the second case study uses a reduced strain range, the third combines data from only two of the three experiments, and the fourth uses a single homogeneous test. The models are investigated and compared based on their accuracy in fitting the selected data and their ability to predict the complete data set.

2 METHODOLOGY

Throughout the investigations, the top ten constitutive models of the ranking study by Marckmann and Verron (2006) are used. Their parameters are identified using data based on Treloar (1944). In the ranked order of the aforementioned study, these are the extended tube, Shariff, micro-sphere, three-term Ogden, Haines-Wilson, Biderman, Hart-Smith, 8-chain, Gent and Yeoh and Fleming models; see Marckmann and Verron (2006) for references.

In order to investigate the hyperelastic constitutive models and their influence on parameter identification in the four case studies, the parameter identification procedure requires definition. Firstly, the experimental data is defined, then the homogeneous numerical method is outlined for comparison to the experimental data and the optimization method is chosen, which includes the optimization algorithm(s) and the choice of error function.

2.1 *Experimental data*

Throughout this study, the digitized form of the homogeneous experimental data of Treloar (1944) from

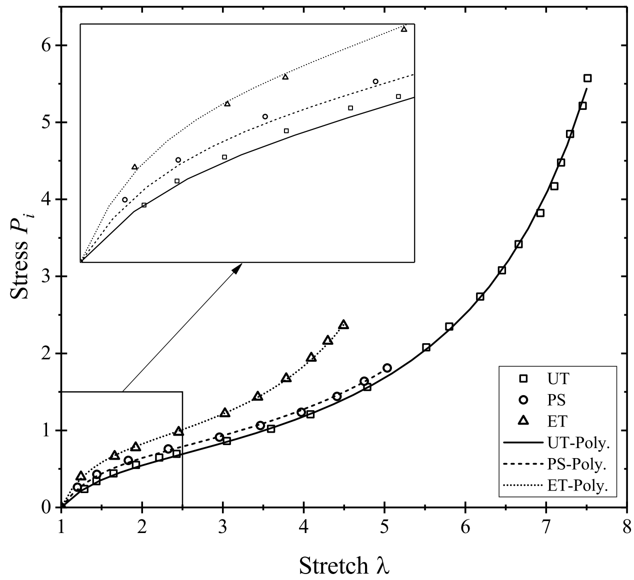

Figure 1: Comparison of Treloar (1944) data from Lopez-Pamies (2010) and fitted 6[th]-order polynomial prediction

Lopez-Pamies (2010) is used, which is defined in terms of the stretch ratio λ_1 and the first Piola-Kirchhoff stress P_1. However, to ensure that the optimization is evenly weighted for each deformation mode across their entire strain ranges, the data is modified. The data sets for each of the three deformation modes are fitted independently with a sixth-order polynomial. From this, twenty-eight equally spaced points are extrapolated for each deformation mode. To assess the validity of this modification, the polynomial fits are compared to the experimental data. These give an average percentage error of 1.35%, 0.8% and 0.48% for uniaxial tension, planar tension and equibiaxial tension fits, which is deemed to be acceptable. The fit is shown in Figure 1.

2.2 *Numerical solutions*

The parameters of each constitutive model are found by minimization of the difference between numerical solutions and the relevant experimental data. For homogeneous experiments, the numerical solutions for all constitutive models (with the exception of the micro-sphere model) may be found by assuming incompressibility and using the general expression

$$P_A = \frac{\partial W}{\partial \lambda_A} + \frac{p}{\lambda_A}; A = 1, 2, 3 \tag{1}$$

Here, P_A and λ_A are defined as previous but in the principal 1, 2 and 3 directions of the Cartesian axes, W is the isochoric strain energy function and p is the hydrostatic pressure. By assuming that the second axis remains consistently unloaded for all homogeneous deformation modes, i.e. $P_2 = 0$, the first Piola-Kirchhoff stress in the direction of the applied load P_1 may be defined as

$$P_1 = \frac{\partial W}{\partial \lambda_1} - \frac{\partial W}{\partial \lambda_2}\frac{\lambda_2}{\lambda_1} \tag{2}$$

This may be used for all constitutive models defined in terms of principal stretches or principal invariants by use of the definitions of the first and second invariants $I_1 = {\lambda_1}^2 + {\lambda_2}^2 + {\lambda_3}^2$ and $I_2 = {\lambda_1}^{-2} + {\lambda_2}^{-2} + {\lambda_3}^{-2}$. Though for convenience, P_1 is also defined for constitutive models given in terms of the Cauchy-Green invariants I_1 and I_2 as

$$P_1 = 2\left[\left(\lambda_1 - \frac{{\lambda_2}^2}{\lambda_1}\right)\frac{\partial W}{\partial I_1} - \left({\lambda_1}^{-3} - \frac{{\lambda_2}^{-2}}{\lambda_1}\right)\frac{\partial W}{\partial I_2}\right] \quad (3)$$

The expressions (2) and (3) are used in conjunction with the assumption of incompressibility, such that $I_3 = \lambda_1\lambda_2\lambda_3 = 1$, to relate the principal stretches for uniaxial, planar and equibiaxial deformations respectively as

$$Uniaxial \qquad \lambda_1 = \lambda;\ \lambda_2 = \lambda^{-\frac{1}{2}};\ \lambda_3 = \lambda^{-\frac{1}{2}} \quad (4)$$

$$Planar \qquad \lambda_1 = \lambda;\ \lambda_2 = \lambda^{-1};\ \lambda_3 = 1 \quad (5)$$

$$Equibiaxial \qquad \lambda_1 = \lambda;\ \lambda_2 = \lambda^{-2};\ \lambda_3 = \lambda \quad (6)$$

The above relations may then be used in the analytical solution of homogeneous experimental predictions for all constitutive models investigated here other than the micro-sphere model.

For the micro-sphere model, the algorithm for the computation of the Kirchhoff stress tensor τ outlined in Miehe et al. (2004) is used. With the same assumption as previous, the Kirchhoff stress in the direction of the applied load τ_1 is calculated using the assumption that $\tau_2 = 0$ to compute the hydrostatic pressure. The Kirchhoff stress τ_1 is then converted to the first Piola-Kirchhoff stress P_1 by $P_1 = \lambda_1\tau_1$.

2.3 *Optimization methods*

In the following case studies the aim is to investigate the ability of the constitutive models to fit and predict the entire strain range of the complete data. The optimization methods therefore do not consider a reduced domain of validity or the omission of data if an appropriate fit is not found, see Marckmann and Verron (2006) if such a method is required.

With the experimental data sets and numerical predictions of the constitutive models defined, these are compared by way of an error function which is minimized to reveal optimal parameters. As a further step to ensure equal weighting throughout the optimization, the relative error E_R is used as the objective function throughout, defined by

$$E_R = \left[\sum_{i=1}^{n}\left((P_{1a})_i - (P_{1d})_i\right)^2\right]^{\frac{1}{2}} \Big/ \left[\sum_{i=1}^{n}{(P_{1d})_i}^2\right]^{\frac{1}{2}} \quad (7)$$

Here, P_{1a} and P_{1d} are the first Piola-Kirchhoff stresses for the analytical model predictions and modified experimental data for n data points respectively. When minimized, this function ensures that the weighting of each data point is independent of stress magnitude.

Due to the capability of predicting the homogeneous experiments with analytical solutions, these solutions are computed within Microsoft Excel. The optimal parameters are then found using the Solver add-in with a nonlinear generalized reduced gradient (NLGRG) optimization algorithm with $10,000$ randomly seeded multi-start parameters. If a global minima is not found, the multi-start population size is increased to $100,000$, which further increases the probability of finding the global minima. This method requires the use of upper and lower bounds, which are determined based on any physical or stability constraints from the original publications of the models, or are otherwise defined based on prior experience. If the method does not locate appropriate minima, the objective function is minimized using Simulia's Isight program and an Adaptive Simulated Annealing (ASA) algorithm with the same upper and lower bounds and the same objective function.

To check that a probable global minima is found, within the constrained problem, the error values are compared across the different homogeneous data set variations. For each model, these checks ensure that the present optimization finds the lowest error for the minimized quantity. For example, if the global minima is found, the error for the first case study using the complete data set will have a lower error magnitude than any of the predictions of the complete data by the other case studies. Similarly, the minimization of a single homogeneous test should have a lower error for that deformation mode than within any of the other case studies, if the global minima is found.

3 RESULTS

The results for each of the case studies are presented individually. For brevity, only the summed relative error for the fitted data and for the prediction of the complete data are given, along with a ranking for the fitted test and the prediction of the complete data. The parameters themselves and other results are omitted since there are a total of one hundred parameter sets.

For most models, a probable global minimum is found using the multi-start NLGRG method with a maximum of $10,000$ multi-starts. Both the Ogden and Haines-Wilson models require an increase in the multi-start population to a maximum of $100,000$. The Shariff model is not compatible with the NLGRG method, which is likely due to the significant difference in sensitivities of its five parameters. Probable global minima were then found for the Shariff model using the ASA algorithm.

From the results of the case studies, it is found that a relative error E_R of less than approximately 0.15 adequately produces a physically realistic response. What is meant by this is that the constitutive model predicts the clear distinction of the different deformation modes and closely predicts the asymptotic behavior at high strains. These phenomenological responses of rubber are shown in Figures 1 and 2. An error of 0.15 is therefore used as a benchmark to assess whether a feasible fit or prediction of the complete data has been obtained.

3.1 *Case study 1: complete data*

The comparative results of the first case study consist of only the constitutive models' fits to the complete data set. The results are given in Table 1 where the models are listed in the order of their ranking from Marckmann and Verron (2006) and a feasible fit is shown in bold, these conventions are followed throughout all case studies.

With consideration of only the error magnitude, it is found that the order here has similarities to the previous ranking study. The extended-tube is the most accurate model, as shown in Figure 2, closely followed by the Ogden and Shariff models. Beyond the Biderman model, the constitutive models fail to exhibit a distinction in the different deformation modes at low and moderate strains but all ten models capably predict the asymptotic behavior.

Table 1: Case study 1 results: error of fitting to complete data set

Model	Fit	Rank	UT	PS	ET
Extended-tube	**0.045**	(1st)	0.014	0.018	0.012
Shariff	**0.053**	(3rd)	0.016	0.018	0.018
Micro-sphere	**0.073**	(4th)	0.030	0.032	0.011
Ogden	**0.052**	(2nd)	0.039	0.006	0.008
Haines-Wilson	**0.098**	(5th)	0.027	0.039	0.032
Biderman	**0.140**	(6th)	0.029	0.034	0.077
Hart-Smith	0.175	(7th)	0.020	0.029	0.126
8-chain	0.276	(9th)	0.054	0.079	0.144
Gent	0.280	(10th)	0.050	0.083	0.146
Yeoh & Fleming	0.193	(8th)	0.024	0.006	0.163

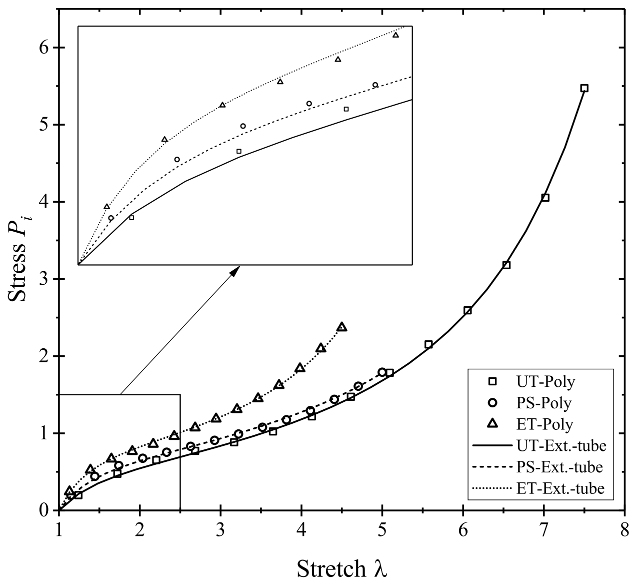

Figure 2: Extended-tube model fitted to modified complete data

3.2 *Case study 2: reduced strain ranges*

The original complete data set is modified by reducing it to 75%, 50% and 25% of the strain ranges in each deformation mode. The results for this study are shown in Table 2. These results show both the error of the fit for each model to the data used in parameter identification and their error in predicting the complete data.

It is found that when predicting the complete data set, the error generally increases as a lower strain range is used. All models provide a realistic response for the 75% strain range, as much as they may be expected to, given the findings of the first case study. However, the only feasible predictions are obtained using a 75% strain range are from the extended-tube and Ogden models. For strain ranges lower than this, physically realistic responses are generally no longer found due to a lack of upturn in the data. This results in an inability to predict the asymptotic behavior.

Across the reduced strain range results, the extended-tube is the best performing model on average, followed by the Ogden and micro-sphere models. However, it is generally evident that predicted responses beyond the experimented strain range are neither reliable nor accurate.

3.3 *Case study 3: two deformation modes*

Using the data from two of the three deformation modes gives three different combinations of reduced experimental data. The results for the fits achieved using the three combinations are given in Table 3. As in the second case study, the error values are shown for the objective function used in identifying parameters and for the error in predicting the complete data set.

The results show that for the most part the ability of a model to accurately fit the data from two deformation modes does not imply a similarly accurate prediction of the third unfitted mode. However, it is found that the test ranking and complete prediction rankings approximately correspond for the combination the combination of uniaxial and equibiaxial tension tests. This combination also gives the lowest average error. The extended-tube model is again generally the most accurate at predicting the complete data set. It is the only model to give a feasible result for all three reduced data combinations.

As well as giving the lowest average error, the combination of uniaxial and equibiaxial tension data gives a feasible fit for five models. Pure shear and equibiaxial tension gives only two feasible fits, and uniaxial tension and pure shear produces a feasible fit for only the extended-tube model.

3.4 *Case study 4: single deformation modes*

In the final case study, the parameters of each model are fitted using the data from a single deformation

Table 2: Case study 2 results: error for the fit to reduced strain range tests and their prediction of the complete data.

	75% Strain range				50% Strain range				25% Strain range			
Model	Test	Rank	Complete	Rank	Test	Rank	Complete	Rank	Test	Rank	Complete	Rank
Extended-tube	0.052	(2nd)	**0.115**	(1st)	0.057	(3rd)	0.492	(3rd)	0.052	(4th)	0.915	(6th)
Shariff	0.054	(3rd)	0.200	(4th)	0.058	(4th)	0.553	(5th)	0.067	(5th)	1.235	(7th)
Micro-sphere	0.062	(4th)	0.738	(10th)	0.061	(5th)	0.317	(1st)	0.044	(1st)	0.482	(1st)
Ogden	0.026	(1st)	**0.120**	(2nd)	0.028	(1st)	0.568	(6th)	0.045	(2nd)	0.765	(4th)
Haines-Wilson	0.087	(5th)	0.238	(5th)	0.055	(2nd)	2.469	(9th)	0.046	(3rd)	16.452	(10th)
Biderman	0.134	(6th)	0.563	(9th)	0.093	(6th)	3.070	(10th)	0.077	(6th)	2.525	(8th)
Hart-Smith	0.152	(7th)	0.382	(6th)	0.127	(7th)	0.481	(2nd)	0.190	(7th)	0.796	(5th)
8-chain	0.337	(9th)	0.463	(7th)	0.386	(9th)	0.688	(7th)	0.311	(9th)	0.643	(3rd)
Gent	0.432	(10th)	0.491	(8th)	0.413	(10th)	0.534	(4th)	0.317	(10th)	0.513	(2nd)
Yeoh & Fleming	0.245	(8th)	0.196	(3rd)	0.280	(8th)	0.895	(8th)	0.254	(8th)	8.006	(9th)

Table 3: Case study 3 results: error for the fit to two of three tests and their prediction of the complete data set

	Uniaxial Tension & Pure Shear				Pure Shear & Equibiaxial Tension				Uniaxial & Equibiaxial Tension			
Model	Test	Rank	Complete	Rank	Test	Rank	Complete	Rank	Test	Rank	Complete	Rank
Extended-tube	0.030	(2nd)	**0.049**	(1st)	0.028	(2nd)	**0.080**	(2nd)	0.025	(1st)	**0.047**	(1st)
Shariff	0.031	(3rd)	0.552	(7th)	0.033	(3rd)	0.233	(3rd)	0.032	(3rd)	**0.059**	(2nd)
Micro-sphere	0.045	(6th)	0.502	(6th)	0.037	(4th)	0.234	(4th)	0.031	(2nd)	**0.085**	(4th)
Ogden	0.032	(4th)	58.837	(9th)	0.011	(1st)	**0.055**	(1st)	0.038	(4th)	**0.072**	(3rd)
Haines-Wilson	0.047	(7th)	1.371E3	(10th)	0.053	(5th)	0.452	(8th)	0.059	(5th)	**0.098**	(5th)
Biderman	0.056	(8th)	0.567	(8th)	0.097	(7th)	0.347	(7th)	0.093	(6th)	0.193	(6th)
Hart-Smith	0.041	(5th)	0.182	(2nd)	0.096	(6th)	0.510	(9th)	0.119	(7th)	0.231	(7th)
8-chain	0.119	(10th)	0.290	(4th)	0.213	(9th)	0.307	(5th)	0.176	(9th)	0.368	(9th)
Gent	0.119	(9th)	0.294	(5th)	0.219	(10th)	0.309	(6th)	0.180	(10th)	0.362	(8th)
Yeoh & Fleming	0.028	(1st)	0.195	(3rd)	0.146	(8th)	0.609	(10th)	0.149	(8th)	0.386	(10th)

mode. The three sets of results are shown for all constitutive models in Table 4, which include the error and ranking of the fit to the single deformation mode and their prediction of the complete data set.

In this case study, the results highlight that a close fit to reduced experimental data does not generally imply an accurate prediction of the complete material response. It is shown that generally the use of a single test in parameter identification is not recommended. The only feasible solutions are both found using the extended-tube model for uniaxial tension and equibiaxial tension tests. This further demonstrates the ability of the extended-tube model to tend towards a physically realistic solution.

4 DISCUSSION

Based on the results of the case studies it is found that the implications of constitutive model selection are strongly correlated with the extent of experimental data used. If a complete data set is available, the choice of constitutive model should be dependent on the model which can most closely fit the data. Although, if time constraints and CPU resources are limited, the Ogden, Haines-Wilson and Shariff models may not be suitable either due to the required modification of the optimization method.

With reduced data, it is again found that the choice of constitutive model determines how accurate a fit may be obtained to the data. However, whether an accurate prediction of the complete response is obtained is shown to be dependent on both the choice of constitutive model and the extent of data used. Generally, it is found that predictions should not exceed the experimented strain range. If only two tests are available, uniaxial tension and equibiaxial tension data (or equivalently uniaxial compression) should be prioritized. These form the bounds of the invariant plane and have been suggested previously to be adequate in providing an acceptable prediction of the overall response for rubber (Latorre et al. 2017). However, this is shown here to also depend on the choice of constitutive model.

Overall the extended-tube model is the best performing model. This model fits a complete data set accurately and generally tends towards physically realistic behavior more than the other models with reduced data. This may be due to the physical origin of its two terms, where one term models the finite extensibility of the rubber molecular chains and the other term models the internal tube-like constraints (Kaliske and Heinrich 1999). However, given that the micro-sphere model is based on similar concepts (Miehe et al. 2004) but does not feasibly predict unfitted deformations, the extended-tube model likely also possesses a mathematical tendency to reproduce this behavior.

Regarding the other models, the Ogden, Shariff and Haines-Wilson models are all phenomenological in nature and are capable of fitting prescribed data accu-

Table 4: Case study 4 results: error for the fit to a single homogeneous test and the prediction of the complete data set

	Uniaxial Tension only				Pure Shear only				Equibiaxial Tension only			
Model	Test	Rank	Complete	Rank	Test	Rank	Complete	Rank	Test	Rank	Complete	Rank
Extended-tube	0.013	(2nd)	**0.055**	(1st)	0.004	(3rd)	0.490	(2nd)	0.009	(6th)	**0.087**	(1st)
Shariff	0.016	(3rd)	200.401	(8th)	0.004	(2nd)	32.792	(8th)	0.010	(7th)	1.277	(7th)
Micro-sphere	0.017	(4th)	7.460E5	(10th)	0.004	(5th)	8.855	(6th)	0.006	(1st)	0.401	(3rd)
Ogden	0.021	(6th)	0.389	(6th)	0.003	(1st)	23.867	(7th)	0.007	(4th)	1.538	(8th)
Haines-Wilson	0.022	(7th)	1.678E4	(9th)	0.017	(7th)	2.134E4	(10th)	0.025	(8th)	45.889	(10th)
Biderman	0.024	(8th)	0.716	(7th)	0.017	(8th)	69.543	(9th)	0.007	(5th)	4.835	(9th)
Hart-Smith	0.018	(5th)	0.212	(2nd)	0.005	(6th)	0.543	(3rd)	0.006	(3rd)	0.352	(2nd)
8-chain	0.031	(10th)	0.338	(5th)	0.055	(9th)	0.627	(5th)	0.034	(9th)	0.448	(5th)
Gent	0.026	(9th)	0.330	(4th)	0.056	(10th)	0.583	(4th)	0.037	(10th)	0.459	(6th)
Yeoh & Fleming	0.008	(1st)	0.249	(3rd)	0.004	(4th)	0.298	(1st)	0.006	(2nd)	0.401	(4th)

rately. However, these should be used only if a depth of experimental data is available. The 8-chain, Gent and Hart-Smith models may not fit the complete data accurately but are found to have lower variance than other models. The equivalence of these models has been observed previously by Chagnon et al. (2004), where they all similarly reproduce the finite extensibility behavior by different mathematical means. The Biderman model does not fit the complete data as accurately as other models and if only reduced data is available the more stable Yeoh form should be preferred (Seibert and Schöche 2000). The Yeoh and Fleming model has four parameters yet fails to accurately fit multiaxial data or predict unfitted deformations.

5 CONCLUSIONS

Parameter identification of hyperelastic constitutive models has been investigated in this study using varying extents of homogeneous experimental data. It is found that the choice of constitutive model determines the effectiveness of a parameter identification method with different implications depending on the extent of experimental data used. In general, with a complete set of experimental data, the choice of constitutive model should be determined based on the most accurate fit to this data. For the experimental data set used, this was the extended-tube model. When a complete set of experimental data is unavailable, a prediction of unfitted behavior is generally not recommended. This is of particular importance to predictions made beyond the experimented strain range. Otherwise, the extended-tube model is shown to generally produce a physically realistic response with a reduced number of experiments and may be used. In this case, uniaxial tension and equibiaxial tension (or equivalently uniaxial compression) tests should be prioritized, since this combination is shown to most capably predict the complete response. These results also indicate that the choice or proposal of a constitutive model should consider its ability to predict unfitted deformations.

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