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UNCERTAINTY QUANTIFICATION IN PREDICTING BEHAVIOUR OF RUBBER-LIKE MATERIALS IN UNI-AXIAL LOADING

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ABSTRACT

Material parameters related to deterministic models can have different values due to variation of experiments outcome . From a mathematical point of view, probabilistic modeling can improve this problem. It means that material parameters of constitutive models can be characterized as random variables with a probability distribution. To this end, we propose a constitutive models of rubber-like materials based on uncertainty quantification (UQ) approach. UQ reduces uncertainties in both computational and real-world applications. Constitutive models in elastomers play a crucial role in both science and industry due to their unique hyper-elastic behavior under different loading conditions (uni-axial extension, biaxial, or pure shear). Here our goal is to model the uncertainty in constitutive models of elastomers, and accordingly, identify sensitive parameters that we highly contribute to model uncertainty and error. Modern UQ models can be implemented to use the physics of the problem compared to black-box machine learning approaches that uses data only . In this research, we propagate uncertainty through the model, characterize sensitivity of material behavior to show the importance of each parameter for uncertainty reduction. To this end, we utilized Bayesian rules to develop a model considering uncertainty in the mechanical response of elastomers. As an important assumption, we believe that our measurements are around the model prediction, but it is contaminated by Gaussian noise. We can make the noise by maximizing the posterior. The uni-axial extension experimental data set is used to calibrate the model and propagate uncertainty in this research.

INTRODUCTION

Uncertainty quantification (UQ) is to consider variation of response of the material in different samples, which results in bounds on the behavioral prediction of the system. UQ plays a pivotal role in modeling under the framework of continuum mechanics. UQ participates in the detection of uncertainty sources and can determine a mathematical model to calculate the error bounds. Usually, in computational modeling, predictions are deterministic due to deterministic methods that researchers use such as least square for parameter calibration. In these methods, a single estimate is calculated based on available data of the system. Although, in real problems, model prediction for a specific

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group of parameters and different combinations of parameter values of model may have similar results. So, one of these combinations is determined in a deterministic approach. However, probabilistic modeling can calculate different combinations of parameters in the form of the probability distribution for model prediction through the propagation of uncertainty. Hence, probabilistic evaluation of computational models can help users to find a model that prediction and input parameters are independent. Another importance of UQ is in the context of safety factor in design that is important, is failure of material. Also, a better estimation of safety factor and cost reduction is the result of generating confidence bounds in probabilistic modeling. The source of uncertainty, generally, are categorized based on their capability in uncertainty reduction, known as "epistemic" which refers to reducible error due to lack of knowledge and we can reduce it by cost and "aleatory" which refers to inherent error of system and we cannot or do not know to reduce. The goal of UQ in computational modeling is the calculation of uncertainty for modeling and prediction. So, quantification process over all uncertainties, in this filed, is uncertainty quantification (UQ) and uncertainty propagation (UP) [1].

Two statistical views, usually, evaluate quantification process; Frequentist view defines probability during a long-term observation based on rate of occurrence, and Bayesian view which considers degree of belief based on the combination of prior knowledge and new data for probability. So, in Frequentist view, parameters are fixed random variables. However, in Bayesian view, parameters are random variables with data. Although wrong prior knowledge can mislead the model, the true definition is helpful in statistical inference. In UQ analysis, uncertainty sources can be categorized because of (1) inherent uncertainty of physical system (2) model parameter uncertainty due to lack of knowledge (3) propagated uncertainty (4) model structure uncertainty because of lack of physics in model. Model uncertainty is the hardest one among all of these sources due to limited knowledge and inaccurate experimental data. On the other hand, one of the attractive fields in computational modeling is modeling of hyper-elastic materials such as elastomers.

Elastomer is a wide meshed cross-linked polymer that behaves entropically elastic and does not show reversible deformation. They are usually classified as filled and unfilled categories. Fillers, in most cases, can reinforce polymers. They increase the stiffness of elastomers; However, they reduce the extensibility of the polymer chains. Manner of elastomers and rubber-like materials shows non-linear behavior, especially during large deformation. Hyper-elastic constitutive models describe the behavior of them in small and large deformation [2–4]. Stress-strain relation is derived from the strain energy function. Hence, researchers spare no efforts to find a strain energy function that captures the behavior of elastomers under different state of loading. Development of constitutive models for cross-linked polymers is hindered by both incompleteness of theoretical approach and limitation in experiment observation. From past decades until now, researchers proposed many models which all of them is lack of uncertainty and are based on deterministic approaches that cause we cannot consider confidence bounds to estimate response of model or reduce uncertainty of system.

There are several hyper-elastic constitutive model from last eighty years. in 1999, Yeoh [5] proposed a new cubic strain energy function based on first invariant. Ogden [6] proposed a model for large deformation in order to remove isotropic and incompressiblity assumptions from constitutive model. James et al. [7], in their work, proposed two analytic forms of strain energy function for isotropic and incompressible materials. Lambert-Diani and Rey [8], in 1998, proposed a family of functions of strain energy associated with hyper-elastic behavior of elastomers. After that, Pucci and Saccomandi [9] reformed Gent model that has a limitation on chain extensibility. They proposed a model that with minimum number of coefficient can capture Treloar data [10]. After one year, Beda and Chevalier [11] combined Gent model and Ogden model to capture experimental data of behavior of rubber like materials. Farhangi et al. [12, 13] investigated the effect of fiber. Valiollahi et al. [14, 15] proposed a stretch-based large deformation method for hyperelastic materials. In 2009, Dargazany et al. [16] proposed a micro-mechanical model that captures inelastic behavior of elastomeric materials such Mullins effect, permanent set and anisotropy. Mohammdai and Bahrololoumi studied on aging of these materials based on this model [17–20]. In 2011, Kroon [21] proposed a model based on eight-chain model by adding some topological constraint of moving space of chain. They showed the performance of their model with experimental data set. In 2016, Nkenfack et al. [22, 23] proposed a new model by adding an integral density and an interleaving constraint part to eight-chain model. Shojaeifard et al. [24, 25] proposed a viscoelastic model and its framework in FEM. Ghaderi et al. [26] proposed a physic-informed neural network model which captures all different state of inelasticity in cross-linked polymer. All of introduced model , in below, have a deterministic approach. Recently, Brewick and Teferra [27] investigated on uncertainty quantification of constitutive model for brain tissue. They consider Ogden model as the reference model in their work. Kaminski and Lauke [28], in 2018, worked on probabilistic aspects of rubber hyper-elasticity. They considered some basic models, from Neo-Hookean to Arruda-Boyce, and showed probabilistic characteristics of them such as expectation, variance, skewness and kurtosis. Also, in last year, Mihai et al. [29] published a paper on uncertainty quantification of elastic materials.

This work presents a parametric stochastic model based on Bayesian model calibration. UQ reduces uncertainties in both computational and real world problems. In this study, we propagate uncertainty through the Caroll model. we believe that our measurements are around the model prediction, but it is contaminated by Gaussian noise. We can make the noise by maximizing the posterior. We train and predict some values based on experimental data set.

The paper is outlined as follows. Experimental test and results are explained in detail in the first section. In section 2, parametric stochastic constitutive model based on Bayesian model calibration are mentioned. Results are showed in section 3. Finally, a conclusion is provided in last section.

Parametric Constitutive Model

Continuum Mechanics

Consider that $\mathbf{X}$ and $\mathbf{x}$ are the reference and current coordinates of an element under deformation $\mathbf{x} = D(\mathbf{X})$ in a body. $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ known as deformation gradient. We can define right Cauchy-green deformation tensor as $\mathbf{C} = \mathbf{F}^T\mathbf{F}$. λ_k and λ_k^2, $k = 1,2,3$, are eigenvalues of $\mathbf{F}$ and $\mathbf{C}$ respectively. The principal invariant of $\mathbf{C}$ mentioned as

$$\begin{aligned}\mathbf{I}_1(\mathbf{C}) &= tr(\mathbf{C}),\\ \mathbf{I}_2(\mathbf{C}) &= \frac{1}{2}((\mathbf{I}_1(\mathbf{C}))^2 - tr(\mathbf{C}^2)),\\ \mathbf{I}_3(\mathbf{C}) &= \det(\mathbf{C}).\end{aligned} \tag{1}$$

Strain energy function can be defined as a function of principle invariants as

$$\Psi = \Psi(\mathbf{C}) = \Psi(I_1, I_2, I_3). \tag{2}$$

First Piola-Kirchhoff stress tensor $\mathbf{P}$ for incompressible materials can be written as

$$\mathbf{P} = \frac{\partial \Psi}{\partial \mathbf{F}} - p\mathbf{F}^{-T}. \tag{3}$$

For incompressible elastomers, $\det\mathbf{F} = 1$ and p is a Lagrange multiplier that arise from the assumption of incompressibility. Here, the hyper-elastic response is characterized by Caroll model [30]. The strain energy density function and uni-axial stress for this model mentioned as follow

$$\Psi = w_1\mathbf{I}_1 + w_2\mathbf{I}_1^4 + w_3\sqrt{\mathbf{I}_2}. \tag{4}$$

By substituting Eq. 4 into 3, one can drive the stress in the loading direction of uni-axial tension test as

$$P^{UT} = \left[2w_1 + 8w_2\left(2\lambda^{-1} + \lambda^2\right)^3 + w_3\left(1 + 2\lambda^3\right)^{-\frac{1}{2}}\right]\left(\lambda - \lambda^{-2}\right), \tag{5}$$

where λ is principal stretch in the loading direction, and w_1, w_2 and w_3 are the model parameters.

Stochastic Modeling

In a model calibration problem, we have n observation and n outputs consisting of

$$[\lambda_{1:n}] = [\lambda_1, \lambda_2, ..., \lambda_n], \qquad [p_{1:n}] = [p_1, p_2, ..., p_n]. \tag{6}$$

Any model can connect inputs λ to p through the use of some parameters W as follow

$$P = f(\lambda; W) = \sum_{j=1}^{m} w_j\phi_j(\lambda) = W^T\blacksquare(\lambda), \tag{7}$$

which j shows the index of parameter, ϕ is basis function and w is the parameter. Caroll model which mentioned in last part is a model with 3 parameters and 3 basis functions. In order to do a stochastic model calibration, we are using Bayesian method.

Bayesian Methodology To calculate joint probability distribution of model parameters that shows uncertainty associated with experimental data, Bayesian model calibration is created. In contrast to least square method that determines best parameters for fitting and does not provide any information regarding parameters' probability, Bayesian method can shows uncertainty of model with stochastic parameters [31]. This method is based on Bayes conditional rule of probability, which is written as

$$\mathscr{P}(W|D,M) = \frac{\mathscr{P}(D|W,M)\mathscr{P}(W|M)}{\mathscr{P}(D|M)}, \tag{8}$$

which W is the vector of unknown model parameters, M is chosen model and D is set of data. $P(W|M)$ known as prior joint distribution and shows degree of believe to the parameters before we know the data. $\mathscr{P}(D|W,M)$ is likelihood joint distribution which describes the observation probability of what we have observed. $\mathscr{P}(W|D,M)$ mentions posterior distribution. $\mathscr{P}(D|M)$ acts as a normalizer, which mentioned as follow

$$\mathscr{P}(D|M) = \int_W \mathscr{P}(D|W,M)\mathscr{P}(W|M)dW. \tag{9}$$

There are two main method for model calibration, Maximum Likelihood Estimation and Maximum Posterior Estimation. These methods are explained in next subsections in detail.

Maximum Likelihood Estimation (MLE) In this method, in order to find parameters, measurement process is modeled by the likelihood function. We believe that our measurement is around the model prediction, but it is contaminated by Gaussian noise. Hence, likelihood function is as follow

$$\mathscr{P}(p|\lambda,W,\sigma)=\mathscr{N}(p|\mathbf{W}^T,\sigma^2), \tag{10}$$

Eq. 10 should be maximized to find model parameters and the noise. So, one can write

$$W_{MLE},\sigma^2_{MLE}=\arg\max\left\{\log\left[\mathscr{P}\left(p|\lambda,W,\sigma\right)\right]\right\}. \tag{11}$$

In veiw of Eq. 11, the solution for W_{MLE} and σ_{MLE} can be calculated as

$$\begin{aligned} W_{MLE} &= (\phi^T\phi)^{-1}\phi^T p, \\ \sigma^2_{MLE} &= \frac{\|\phi W_{MLE}-p\|^2}{n}. \end{aligned} \tag{12}$$

Hence, after solving the problem, we can calculate median and bounds with two standard deviation of model parameters as follows

$$\begin{aligned} m(\lambda) &= W^T_{MLE}\phi(\lambda), \\ l(\lambda) &\approx m(\lambda)-2\sigma_{MLE}, \\ u(\lambda) &\approx m(\lambda)+2\sigma_{MLE}. \end{aligned} \tag{13}$$

Maximum Posterior Estimation (MPE) In this method, in order to find parameters, measurement process is modeled using the posterior. We believe that our measurement is around the model prediction, but it is contaminated by Gaussian noise. So, we have the same likelihood as Eq. 10. The difference of this method with last method is that here posterior should be maximized instead of likelihood function. We model the uncertainty in model parameters using a prior. Before we see the data, we believes that the weights are around zero with a given precision as follow

$$\mathscr{P}(W|\alpha)=\mathscr{N}(W|0,\alpha^{-1}\mathbf{I})=(\frac{\alpha}{2\pi})^{\frac{m}{2}}\exp\Big(-\frac{\alpha}{2}\|W\|^2\Big), \tag{14}$$

which α acts as a regularizer that kills overfitting. The posterior summarizes our state of knowledge after observing data, if we know the precision parameter and the noise variance. We can write posterior for our problem based on Eq. 8 as follow

$$\mathscr{P}(W|\lambda,p,\sigma,\alpha)=\frac{\mathscr{P}(p|\lambda,W,\sigma)\mathscr{P}(W|\alpha)}{\int\mathscr{P}(p|\lambda,W,\sigma)\mathscr{P}(W|\alpha)dW}. \tag{15}$$

So, solving optimization problem to maximize posterior can calculate W_{MPE} as follow

$$W_{MPE}=argmax\log\mathscr{P}(p|\lambda,W,\sigma)\mathscr{P}(W|\alpha), \tag{16}$$

if likelihood and prior are Guassian, we can say

$$\log\mathscr{P}(p|\lambda,W,\sigma)=-\frac{1}{2\sigma^2}\|\phi W-p\|^2-\frac{\alpha}{2}\|W\|^2, \tag{17}$$

solution for W_{MPE} can mentioned as

$$W_{MPE}=(-\sigma^{-2}\phi^T\phi+\alpha\mathbf{I})^{-1}\phi^T p. \tag{18}$$

To make new prediction with new inputs, we can use as follow equation

$$\mathscr{P}(p_{new}|\lambda_{new},W_{MPE},\sigma)=\mathscr{N}(p_{new}|W^T_{MPE}\phi(\lambda_{new}),\sigma^2). \tag{19}$$

Median prediction, lower bound and upper bound are calculated as follow

$$m(\lambda)=W^T_{MPE}\phi(\lambda),\quad l(\lambda)\approx m(\lambda)-2\sigma,\quad u(\lambda)\approx m(\lambda)+2\sigma. \tag{20}$$

Also, posterior function is written based on multivariate normal distribution as follow

$$\begin{aligned} &\mathscr{P}(W|\lambda,p,\sigma,\alpha)=\mathscr{N}(W|m,\mathbf{S})= \\ &\det(2\pi\mathbf{S})^{-\frac{1}{2}}\exp\left[-\frac{1}{2}(W-m)^T\mathbf{S}^{-1}(W-m)\right], \end{aligned} \tag{21}$$

which $m=\sigma^{-2}\mathbf{S}\phi^T p$ is mean, and $(\sigma^{-2}\phi^T\phi+\alpha\mathbf{I})^{-1}$ is covariance matrix.

Results

Experimental Tests

In this part, measurement method for hyper-elastic deformation, setup and techniques are described. A uni-axial test is implemented for two materials, silicon and polyurethane based adhesives. Four specimens are used for each material.

From a same batch, each sample had a dumbbell shape. Each sample was cast based on standard dimension (ASTM D412- Die C) in Fig. 1.

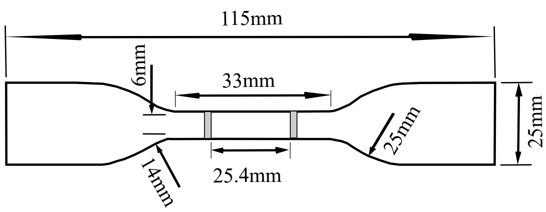

FIGURE 1. Detailed sample dimensions

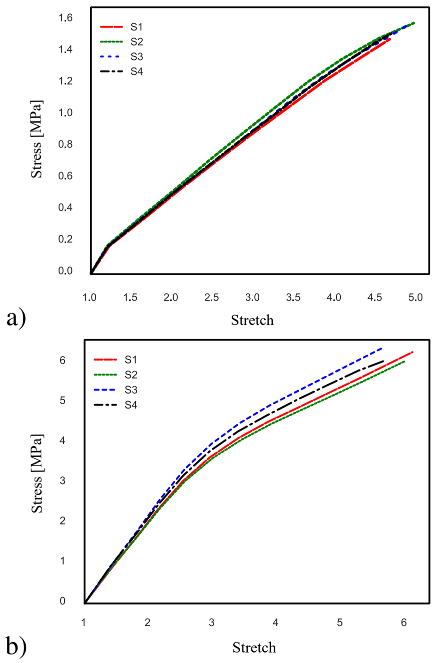

FIGURE 2. Stretch Stress results of mechanical tests for a) DC b) PUB

Quasi-static tensile tests were conducted on a uni-axial universal Testing Machine (TestRecources 311 Series Frame). Samples are clamped between two grips with a loading at rate of $25mm/min$ at room conditions (i.e. $22 \pm 2°C, 50 \pm 3\%RH$). Measurement is conducted by an external extensometer. The stress-strain curves of each samples for DC and PUB is shown in Fig. 2.

Model Calibration and Prediction

In order to show uncertainty quantification and prediction of Caroll model with two observed date set, a model calibration is conducted by MPE and MLE methods. Fig. 3 and Fig. 4 show the results for PUB and DC respectively.

CONCLUSION

In this paper, we introduced a probabilistic constitutive model for cross-linked polymers. This model is based on the

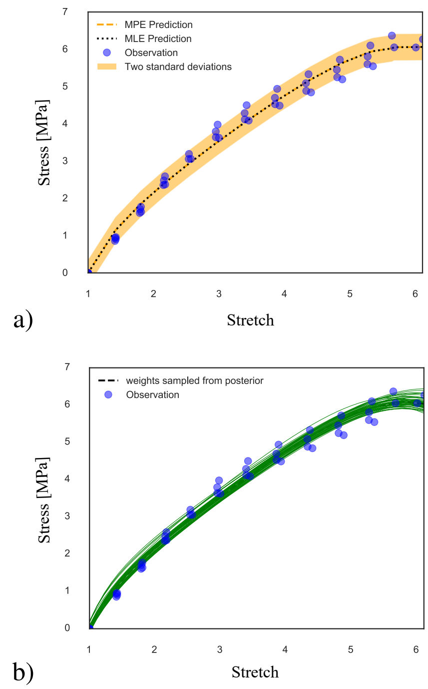

FIGURE 3. Model calibration of Caroll model for PUB a) prediction b) plausible models

Bayesian model calibration such that we maximize likelihood and posterior to see the effect of them. We employed this approach and Caroll model to indicated performance and difference of MPE and MLE by using several experimental data on PUB and DC in uni-axial. In the future, we are going to us a non-parametric approach for proposing a probabilistic constitutive model which shows epistemic and aleatory uncertainty.

Multivariate Normal Distribution

The probability density function (pdf) of a multivariate normal distribution, with a random vector $\lambda = (\lambda_1, \lambda_2, ..., \lambda_n)$, mean $\mu = (\mu_1, \mu_2, ..., \mu_n)$ and positive-definite covariance matrix $\mathbf{S} = [\sigma_{ij}]$, can be written as

$$P(\lambda|\mu,\mathbf{S}) = \frac{1}{(2\pi)^{\frac{n}{2}} \mid \mathbf{S} \mid^{\frac{1}{2}}} \exp\left[-\frac{1}{2}(\lambda-\mu)^T \mathbf{S}^{-1}(\lambda-\mu)\right]. \quad (22)$$

Multivariate normal distribution plays a crucial role in multivariate statistical analysis and has wonderful properties. For example, summation of some multivariate normal distribution has normal distribution and their product has log-normal distribution. If $\mu = 0$ and $\mathbf{S} = \mathbf{I}$, it is called standard normal distribution. To gain a better insight to the distribution a bivariate normal distribution is showed in Fig. 5.

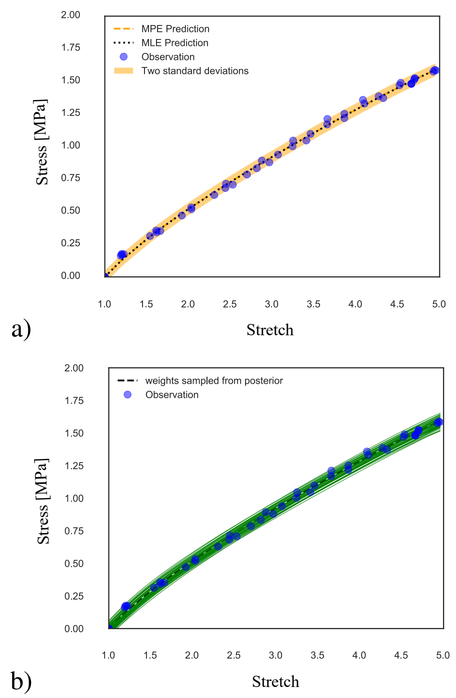

FIGURE 4. Model calibration of Caroll model for DC a) prediction b) plausible models

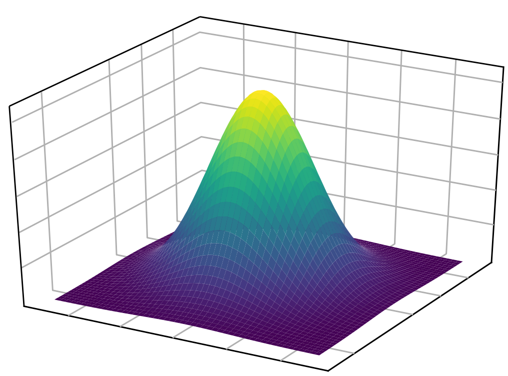

FIGURE 5. Schematic illustration for bivariate normal distribution

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