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Parameter identification study of frequency response data for a trilayer conjugated polymer actuator displacement model

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Abstract

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Keywords

trilayer, actuator, response, frequency, model, displacement, polymer, study, conjugated, parameter, data, identification

Disciplines

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Parameter Identification Study of Frequency Response Data for a Trilayer Conjugated Polymer Actuator Displacement Model

Emmanuel D. Blanchard, Mitchell J. Smith, and Chuc H. Nguyen

***Abstract*— This article investigates the effect of three uncertain parameters on a model of conjugated polymer actuators. These uncertain parameters are the diffusion coefficient (*D*), the resistance (*R*), and the double-layer thickness (δ). The model sensitivity to these parameters is analyzed and a parameter estimation study is performed using artificially generated data as well as laboratory yielded experimental measurements. The parameter estimation method used in this article is based on a Bayesian cost function, and gives us an insight on how much the estimation can be trusted, which is useful information for the design of controllers. Results indicate that for stochastic controllers to be designed effectively using this model, the resistance is the best known parameter and should therefore be designed for with greater confidence in its value, while the controller should be more robust with respect to the diffusion coefficient and the double-layer thickness. However, significant discrepancies between the model and its reduced form used for control purposes seem to indicate that a better suited model would be needed to start developing stochastic controllers.**

I. Introduction

Recent research into polymeric materials has led to the requirement of reliable prediction models and robust control of Electro Active Polymers (EAP's) as actuators. The credit for the discovery of EAP's is given to Roentgen, who in 1880, experimented with an electro-activating rubber-band to move a cantilever with a mass attached to the free-end [1]. Since the 1970s academic and industrial interest in EAP applications has sparked research and has increased the list of EAP materials available. The bulk of work focused on the prediction and control models were developed post 1990 [1-3].

Applications of EAP's are contained in many different areas. Some applications include its use as part of electrochromic "smart" glass, as one component in the photoreceptors of electrophotographic and xerographic devices, and as thin flexible shaped batteries [4, 5]. Of particular interest is their potential use as an actuator or sensor in a biomimetic situation, commonly referred to as an artificial muscle. One particular group of EAP's known as Conjugated electro active Polymers (CPs) have been attracting the attention of researchers in the past decade. This is mainly due to the features that make them attractive for applications including low power consumption, light weight, simple construction and noiseless operation [6]. In particular CPs based on pyrrole, thiophene and aniline are the focus of current research. Polypyrrole (PPy) and polyaniline are two of the most commonly used CPs for actuation [7-8].

In order to utilize these EAPs in any application it is highly desirable to have predictive models available for feasibility studies, design optimization, and precision control. Until recently the control and control-oriented modeling of CPs had been largely unexplored [9]. Original work by J.D.W. Madden [10] and later extended by Fang et al. [11] has led to a model for robust control of CP actuators. These both present a transfer function mathematical model for predicting the bending behavior of EAPs. The latter work goes on to describe a self-tuning regulator which utilizes a parameter projection (in the time domain) step for robust control; this is required because of the relatively short time frame in which the parameters stay constant. Without this parameter estimation step the prediction model becomes inaccurate and results in imprecise control due to the parameters' value expiring. This remedies the previously reported problem of non-repeatability of experiments.

In this paper, a parameter estimation study using frequency response data for the artificial muscle model developed by Madden [10] and used in Fang et al. [9, 11] is performed, and a sensitivity analysis is included. Parameter estimation is performed on real data taken from prior experiments after checking the validity of the method on artificially generated data.

II. Electro-Chemo-Mechanical Modeling of a Trilayer CP Actuator

A. The Infinite-Dimensional Model

The work of Fang et al. [11] extends the diffusive-elastic-metal model of Madden [10] for a trilayer conjugated polymer actuator. The model used in [11] combines both the electrochemical and the mechanical dynamics and is thus known as an electro-chemo-mechanical model. The model for the displacement of the actuator is presented in three modules: electrical admittance, electromechanical coupling and mechanical output. The admittance module relates the input voltage to a current flowing through the system. The electromechanical coupling then relates the current in the system to an electrically induced strain and charge density. The final mechanical output module relates the electrically induced curvature to the geometric curvature, thus giving the displacement, as shown in Fig. 1.

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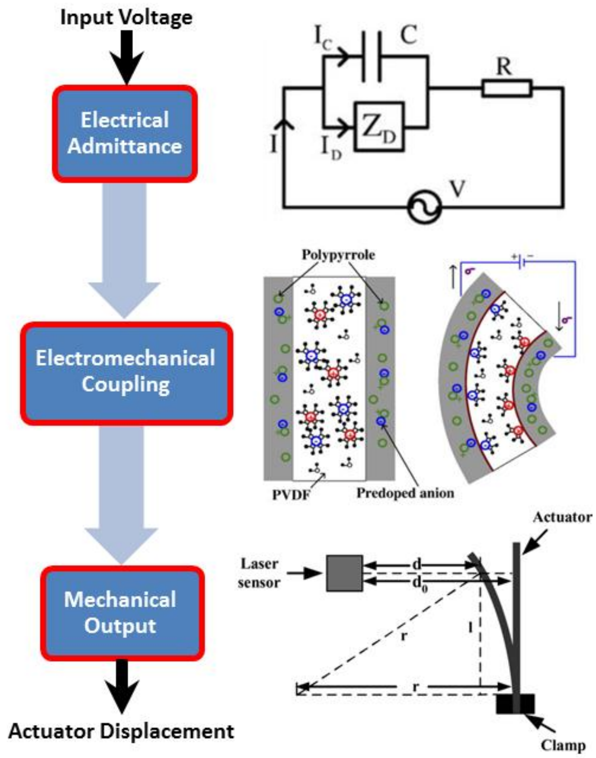


Fig.1. Three distinct modules that form the actuator displacement mathematical model (figure adapted from various figures in [11])

The voltage-to-displacement transfer function model is given by,

$$G(s) = \frac{y(s)}{V(s)} = \frac{1}{2} \times \frac{C_m\, C}{R\, C\, s + \dfrac{1}{1 + \dfrac{1}{\delta}\sqrt{\dfrac{D}{s}}\tanh\left(h\sqrt{\dfrac{s}{D}}\right)}} \tag{1}$$

where

$$C_m \overset{def}{=} \frac{3\,\alpha\, l^2 \left[\left(1 + \dfrac{h}{h_{pvdf}}\right)^2 - 1\right]}{8\, h_{pvdf}\, h W L \left[\left(1 + \dfrac{h}{h_{pvdf}}\right)^3 + \dfrac{E_{pvdf}}{E_{ppy}} - 1\right]} \tag{2}$$

and where (more details can be found in [11])

y(s) is the Laplace transformed displacement function

V(s) is the Laplace transformed voltage function

R is the electrolyte and contact resistance

D is the diffusion coefficient for modeling the diffusion of ion concentration

δ is the double-layer thickness, or Helmholtz double-layer

h is the thickness of the polymer (PPy) layer

C is the double-layer capacitance at the polymer-electrolyte interface

α is the charge-to-strain ratio

l is the distance from the clamped end to the laser incident point when the actuator is at rest

h_{pvdf} is the thickness of the polyvinylidene fluoride (PVDF) layer

W is the width of the PPy layer

L is the length of the PPy layer

E_{ppy} is the modulus of elasticity for the PPy layer

E_{pvdf} is the modulus of elasticity for the PVDF layer

B. *Reduced Finite-Dimensional Model*

The work of Fang et al. [11] also presents a (second-order) reduced form of the model. Indeed, due to the hyperbolic tangent term, the infinite-dimensional system is not suitable for real-time control purposes and is therefore approximated by

$$G(s) \approx \frac{C_m\, C}{R\, C\, s + \dfrac{1}{1 + \dfrac{2\,D}{h\,\delta}\displaystyle\sum_{n=0}^{N} \dfrac{1}{s + \pi^2\,(2n+1)^2\, D\,(2h)^{-2}}}} \tag{3}$$

where N is the number of terms taken in the series approximation.

For typical parameter values such as the values shown in Table 1, using $N = 1$ for (3) is a good approximation of (1), especially at low frequencies, which results in the third order system

$$G(s) \approx \frac{b'_1\, s^2 + b'_2\, s + b'_3}{s^3 + a'_1\, s^2 + a'_2\, s + a'_3} \tag{4}$$

where the coefficients b'_1, b'_2, b'_3, a'_1, a'_2, and a'_3 can be written in terms of the physical constants [11].

TABLE I. TYPICAL PARAMETER VALUES OF THE MODEL

Parameter	Value	Parameter	Value
D	2×10^{-10} m² s⁻¹	E_{pvf}	440 MPa
R	15 Ω	E_{ppy}	80 MPa
δ	25 nm	L	20 mm
C	5.33×10^{-5} F	l	15 mm
h	30 µm	W	5 mm
α	1.3×10^{-10} m³ C⁻¹	b	170 mm

For typical parameter values such as the values shown in Table 1, the third pole and the second zero have a different order of magnitude than the first two poles and the first zero, respectively [11], and can therefore be ignored, which yields a second-order system with one zero and two poles,

$$\hat{G}(s) \approx \frac{b_1\, s + b_2}{s^2 + a_1\, s + a_2} \tag{5}$$

where the coefficients b_1, b_2, a_1 and a_2 can be written in terms of the physical constants [11]. A comparison of the full model, the third-order model and the second-order reduced model is illustrated in [12].

III. Sensitivity of the Model to Parameter Variation

Three parameters are considered uncertain. The diffusion coefficient D and the electrolyte and contact resistance R are uncertain due to the fact that they depend on external conditions. D tends to vary more due to the fact that it decreases due to solvent evaporation which hinders the diffusion of ions. This is the main reason for the very large variability of D. The double-layer thickness, δ, is a fixed parameter, but is also treated as uncertain due to the fact that its size is very small (~25 nm) and cannot be measured very precisely. The expected ranges of these three uncertain parameters are given in Table 2.

TABLE II. Physically Meaningful Values for the Uncertain Parameters

Parameter	Minimum Value	Maximum Value
D	1×10^{-14} m^2 s^{-1}	2×10^{-10} m^2 s^{-1}
R	15 Ω	100 Ω
δ	20 nm	100 nm

A sensitivity analysis was performed by plotting Bode plots for different values of the uncertain parameters for both models. These results indicated that D caused both of the models to vary the most. This could be a direct result of the large range of typical physical values ($D \epsilon$ [1×10^{-12}, 1×10^{-8}] m^{2}s^{-1}). The sensitivity of Bode plots to variation in the diffusion coefficient variation D is shown in Fig. 2 (for the reduced model) and Fig. 3 (for the full model). It was found that lower values of D caused large discrepancies between the two models. It was observed up to 40 dB difference between the two models' magnitude plots and up to 40 deg difference in the phase plots.

Further to this, R and δ are roughly equal in the influence of their value on the behavior on the model. More details and figures can be found in [12], where the sensitivity analysis results and implications are used as a means of "checking" the estimated parameter values, which is achieved by assessing the consistency of the parameter estimation results with the results observed when plotting the Bode plots for different values of the uncertain parameters.

Variations of R were found to cause a variation in the models much less than that of D. The observations were taken for R varying between 1 Ω and 100 Ω. Correspondingly lower values of differences between the two models were also observed for R. It was found that lower values of R caused the largest discrepancies between the two models. It was observed up to 20 dB difference between the two models' magnitude plots and up to 20 deg difference in the phase plots.

The smallest variations in the model due to a varying parameter were observed for δ. The observations were taken for δ varying between 1 nm and 100 nm. Correspondingly lower values of differences between the two models were also observed for δ. It was found that lower values of δ caused the largest discrepancies between the two models. It was observed up to 10 dB difference between the two models' magnitude plots and up to 10 deg difference in the phase plots.

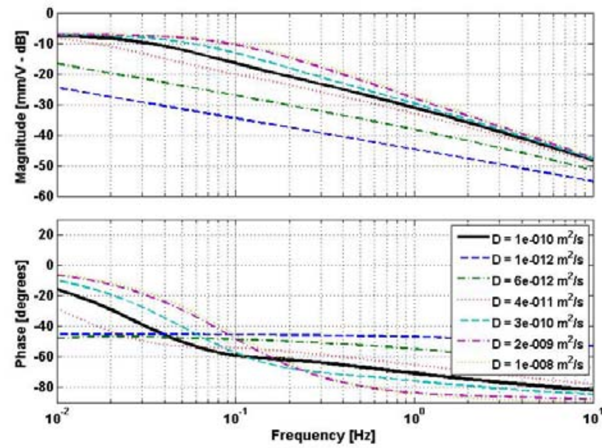


Figure 2: Sensitivity of Bode plot to variation in the diffusion coefficient using the reduced model

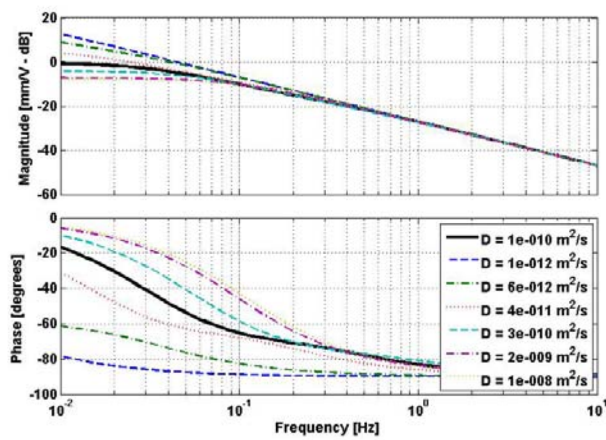


Figure 3: Sensitivity of Bode plot to variation in the diffusion coefficient using the full model

IV. Parameter Estimation Using Frequency Response Data

A. Choice of Parameter Estimation Method

A Bayesian approach to parameter estimation is used. The simulation involves the formation of a multi-dimensional grid, calculating the value of the cost function at every point considered, and finding the minimum of those calculated values. The main advantage of this parameter estimation is that the quality of the maximum likelihood estimate is related to the shape of the Bayesian cost function, with a sharp minimum indicating an accurate estimate [13]. This will be useful in order to design better controllers for artificial muscles. Adaptive controllers are typically designed based on estimates for the uncertain parameter without information on how reliable these estimates are. This is especially a problem when dealing with non-identifiability issues, i.e. when several combinations of values for the uncertain parameters basically yield the same responses. In these cases, stochastic controllers should be designed instead, using a range of possible values for these uncertain parameters and trying to obtain the best average answer since the actual values of these parameters cannot be known. Some parameters might still have estimates which can be trusted while others cannot. This can be visualized when looking at the shape of the Bayesian cost function. The cost function can yield very similar values when a first parameter varies (this parameter is unidentifiable) while it yields very different values when another (identifiable) parameter varies, as explained in [13]. In that case, the stochastic controller would only need to take the parameters that cannot be estimated into account.

For greater precision, MATLAB's constrained minimization function ("fmincon") was used. This involves providing an initial estimate and bounds to constrain the problem. The results from the grid simulation are used as the initial estimate, and bounds proportional to these results were used as the bounds. The parameter estimation method has been tested with a number of sets of artificially generated data obtained by introducing white noise in to the model [12]. It was observed that the recovery of the input parameter values was marginally better when the full model was used to generate the artificial data [12]. The parameter estimation was then conducted using real experimental data from a PPy conjugated polymer actuator sample from a laboratory.

B. Choice of Cost Function

A traditional choice of cost function is the sum of square residuals in the ordinates only (6), that is the sum of the square of the differences between the observed and predicted "*y-values*". This choice is unsuited to this particular inverse problem because a method of combining the cost function for both the magnitude and phase results is needed. This disregards that the two plots are linked as the two plots are a graphical representation of one complex number.

$$\varepsilon \overset{def}{=} \sum_n w_M \left|M\left(j\omega_n;R;D;\delta\right)-M_n\right|^2 + w_\phi \left|\phi\left(j\omega_n;R;D;\delta\right)-\phi_n\right|^2 \quad (6)$$

where

ω_n is the n-th discrete frequency at which the magnitude and phase measurements were taken

$M\ (j\omega_n;\ R;\ D;\ \delta)$ is the simulated magnitude data using particular parameter values for R, D and δ. Either of the full or reduced model can be used here.

M_n is the n-th magnitude measurement

w_M is the weight for the magnitude residuals. This needs to be chosen so that its units are the reciprocal of the units of M and so that equal priority is given to both M and ϕ

$\phi\ (j\omega_n;\ R;\ D;\ \delta)$ is the simulated magnitude data using particular parameter values for $R;$ D and δ. Either of the full or reduced model can be used here.

ϕ_n is the n-th phase measurement

w_ϕ is the weight for the phase residuals. This needs to be chosen so that its units are the reciprocal of the units of ϕ and so that equal priority is given to both M and ϕ

For this reason alone it is far more mathematically rigorous to choose a cost function that represents the difference between the observed complex number and the predicted complex number. In effect this would mean that the process would be "*curve-fitting*" the Nyquist plot of the measured experimental data with either or both of the full and reduced models. That is, the cost function is defined as

$$\varepsilon \overset{def}{=} \sum_n \left| G\left(j\omega_n;R;D;\delta\right) - M_n \exp\left(j\phi_n\right)\right|^2 \quad (7)$$

where $G(j\omega_n;\ R;\ D;\delta)$ is the simulated data using particular parameter values for R, D and δ. Either of the full model or reduced model can be used here.

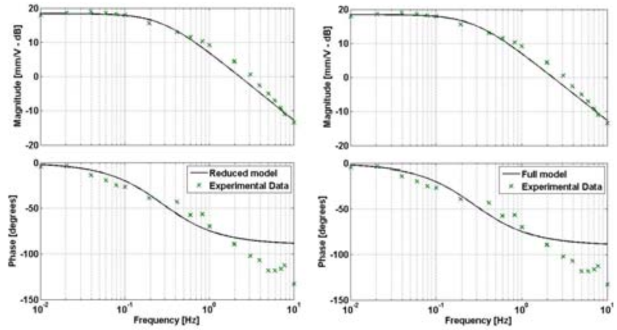
C. Results

Results for both the reduced model and the full model are displayed in Table 3, which shows that the difference between the estimates for each of the two models is quite large. The full model is not suitable for real-time control purposes. However, looking at discrepancies between the two models shows that the estimates of the uncertain parameters might not necessarily result in good controllers even if the Bayesian cost functions have sharp minima indicating accurate estimates. Controller gains would be calculated based on these estimates, but the fact that the reduced model would yield different estimates would mean that the controller (which is based on a second degree model) would have an effect on the system somewhat different than what we might expect. Therefore, this parameter estimation study shows us that there might be great room for improvements of the control performance obtained in [11] by using a more adapted model. Note that the value of the estimate of R is out of the range shown in Table 2. Had this estimate been forced to stay in that range, the estimated value of R would the lowest value in that range.

TABLE III. ESTIMATES FOR THE UNCERTAIN PARAMETERS FOR THE LABORATORY RECORDED DATA

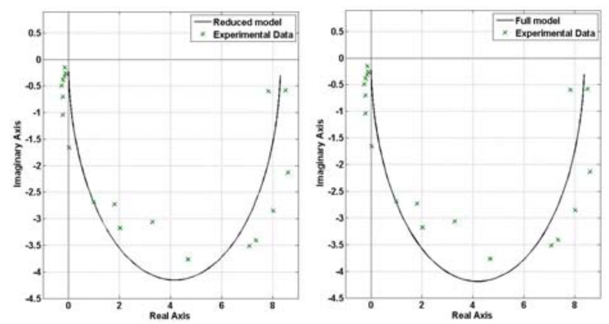
Parameter	Reduced Model	Full Model
D	4.734×10^{-10} m^2 s^{-1}	6.788×10^{-10} m^2 s^{-1}
R	0.573 Ω	0.348 Ω
δ	50.31 nm	20.74 mm

Both the full and reduced models were able to produce equally good fits to the experimental data, though neither was able to capture the high frequency phase behavior, with the measured lag being below the model asymptote (see Fig. 4 and Fig. 5). It shows that this model is not adapted for high frequencies.



(a) **(b)**

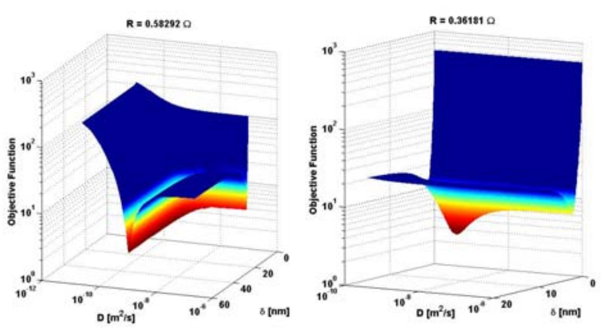
Figure 4: Bode plot results (at the minimum point) for the laboratory recorded data; (a) Reduced model; (b) Full Model



(a) **(b)**

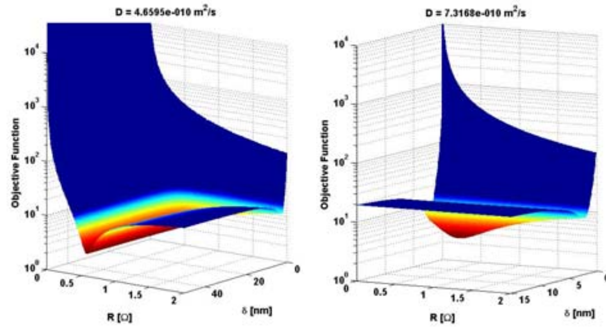
Figure 5: Nyquist plot results (at the minimum point) for the laboratory recorded data; (a) Reduced model; (b) Full Model

Non-identifiability issues for each model were observed through plotting the cost function for all the values considered in the multi-dimensional simulation grid. This revealed that non-identifiability issues exist for both the full and reduced models as evidenced by the long troughs that appear in the plots of the cost function. On this note, Fig. 6 and Fig. 7 show signs that δ is non-identifiable for the reduced model while Fig. 8 shows that D is non-identifiable for the full model.



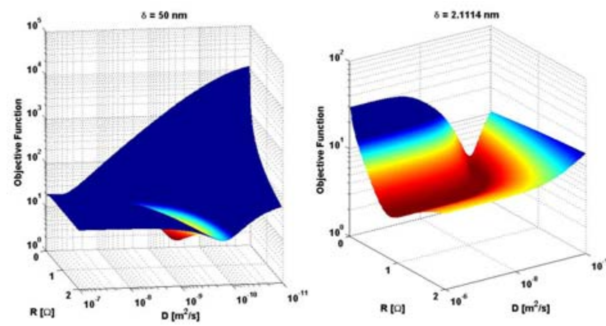
(a) **(b)**

Figure 6: Cost function plot results around the minimum point at fixed R for the laboratory recorded data; (a) Reduced model; (b) Full Model



(a) **(b)**

Figure 7: Cost function plot results around the minimum point at fixed D for the laboratory recorded data; (a) Reduced model; (b) Full Model



(a) **(b)**

Figure 8: Cost function plot results around the minimum point at fixed δ for the laboratory recorded data; (a) Reduced model; (b) Full Model

The observed output values from the parameter estimation results with the exception of R were within accepted ranges of typical physical experimental values. The estimates for the resistance parameter R, for both models, indicated a very low resistance. This does not seem very realistic because it would imply a high current. This may be the result of unmodeled high frequency dynamics or perhaps inaccurate values were used for the other model parameters not estimated in the study. A method of measuring this parameter value should be developed to test whether such a low resistance is physically sensible.

From the sensitivity analysis it was concluded that D affects the behavior of both of the models more than R and δ [12]. It was also found that while the reduced model and full model agree well for many combinations of the parameters, the reduced model shows some significant deviations from the full model. The observation that δ is non-identifiable for the reduced model agrees with the implications of the sensitivity analysis; since δ was found to not have a strong influence on the behavior of the model, a range of δ values would yield similar results. In contrast the diffusion coefficient D shows slight signs of non-identifiability when using the full model, which seems to contradict the implications from the sensitivity analysis that D is the most influential parameter on the shape of the Bode plot. A possible explanation is that D becomes less influential on the full model as it increases in its value, as observed in Fig. 2 and Fig.3.

The parameter estimation solution technique was also tested with a number of sets of artificially generated data (containing added white noise). It was observed that the recovery of the input parameter values was marginally better when the full model was used to generate the artificial data. This was coupled with both the full and reduced models yielding approximately equal quality of fits as evidenced by the similar values of the minimum objective function point [12]. A similar issue of non-identifiability of the diffusion coefficient D was observed using the test data and the full model for estimating the parameters.

The implications from the results obtained in the analysis of the parameter estimation results are that in a conservative design of controllers the value of R is the only parameter (of the three studied) that can be designed for confidently, though the value found was not physically sensible. Further research could be directed at developing a method to measure the resistance parameter. The results also show that D and δ would need further study to estimate confidence intervals around the estimated value so that controllers' designs can be adequately conservative. A study in to achieving confidence intervals for the parameters estimated would require more sophisticated parameter estimation techniques.

V. CONCLUSIONS

The objective of this study was to find non-identifiability issues using the tri-layered conjugated polymer actuator displacement model used in [11] in order to treat estimates that can be trusted as deterministic and use stochastic formulations when dealing with estimates that cannot be trusted (when the Bayesian cost function has an entire region of minima, e.g., a line or a valley). The three uncertain parameters are the diffusion coefficient (D), the resistance (R), and the double-layer thickness (δ). The parameter estimation method used in this study was a Bayesian approach similar to the one developed by Blanchard et al. [13, 14] which has been proven to identify zones of non-identifiability [13]. Since the full model used in [11] is not suitable for real-time control purposes, it is approximated by a reduced form (second-order) of the model [11].

Results indicate that for stochastic controllers to be designed effectively using this model, the resistance is the best known parameter and should therefore be designed for with greater confidence in its value, while the controller should be more robust with respect to the diffusion coefficient and the double-layer thickness. However, the fact that the two models yield different non-identifiability issues clearly indicates that a better suited model would be needed to start developing stochastic controllers. The positive aspect is that there seems to be room for great improvement of control performances by using better suited models in the future. The parameter estimation method used in this paper has been proved to retrieve results with noise using artificial data [12] and this technique could therefore also be extended to other models that exist in the literature. It seems probable that the biggest problem with the model used in this paper was the discrepancy between experimental data and the model at high frequencies.

Future work will include replacing this model by a more recent one that is better suited for high frequencies, such as the model developed by Nguyen et al. [15]. Preliminary results have been obtained and point out to better results indicating that the use of stochastic controllers would make more sense using that model. Future work will also include the use of the polynomial chaos theory coupled with the Bayesian approach. Typical runtimes for the resolutions shown in Figs. 6-8 (grids of 200x200x200) were between 15 and 30 minutes. With the polynomial chaos theory, results for a similar resolution would probably easily be obtained within a few seconds or even less [13, 14], which would also enable the use of higher sample frequencies if needed.

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