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An effective inverse procedure for identifying viscoplastic material properties of polymer Nafion

Wei Zhang, Chongdu Cho *, Yang Xiao

Department of Mechanical Engineering, Inha University, Incheon 402-751, South Korea

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ABSTRACT

An effective inverse procedure is suggested to identify the viscoplastic material properties of polymer Nafion, by minimizing differences in the force–displacement responses of uniaxial tension test between experimental and simulation results. In this procedure, a two-layer viscoplastic constitutive model is adopted to describe the viscoplastic behavior of Nafion. A response surface method is used as a forward solver to calculate the force–displacement response for given material property varying continuously in a certain range. An intergeneration projection genetic algorithm (IP-GA) is then employed as the inverse operator on the response surface to determine the unknown key constants. The selected viscoplastic constants, *A*, *n* and *f*, are varied iteratively using the proposed inverse procedure until the stopping criterion is satisfied. The identification results for two cases demonstrate the effectiveness of the present inverse procedure, as well as its robustness to the noises effects. It is found that this procedure is a potentially useful tool to effectively help determine the viscoplastic material properties of polymer Nafion.

1. Introduction

Polymer Nafion has a very complex material property for its mechanical behavior which has interested scientists and engineers for many years, especially at present when it is widely applied to fuel cells. As one of the most important components in the membrane electrode assembly (MEA), Nafion has a significant contribution to mechanical durability of the fuel cell. Some studies [1–3] show that stress responses of Nafion might play a key role in the durability. To acquire such responses, simulation technique such as finite element analysis (FEA) is probably considered as the best tools. Several simulation models of Nafion have been developed to predict stress responses to complement experimental studies. In order to ensure accurately predicted stress responses using simulation techniques, accurate material properties are necessary.

Although various types of constitutive models e.g. linear elastic model [4,5], linear elastic perfectly plastic model [6,7], viscoelastic model [8,9], hyperelastic [10], etc. have been developed to describe the material properties of Nafion, it is still not very clear how the stress response changes in different working environments. Furthermore, while these models met with some success to roughly estimate the stress responses, an appropriate viscoplastic model is needed to accurately predict stress values. This is because the irreversible behavior, when the material undergoes large and plastic strains and therefore viscoplastic flow, requires a viscoplastic model to build an accurate constitutive model.

Among existing viscoplastic models [11–13], a two-layer viscoplastic model [14] offers a nonlinear framework to cope with the viscoplastic behavior of Nafion with variation of time, temperature and humidity. This model is already incorporated into the commercially available finite element software ABAQUS [15], and hence, it is very convenient to be used to calculate the stress responses. This model mainly consists of an elastic–plastic network and an elastic–viscous network. A brief introduction is given in Appendix A at the end of this paper. In elastic–plastic network, elastic–plastic constants such as initial yield strength and yield strain can be easily determined by using the stress–strain relationship that calculated from the force displacement (FD) data recorded during the tensile testing. However, some key viscoplastic constants such as *A*, *n* and *f* in the elastic–viscous network are difficult to directly determine using measured FD response curve. To deal with it, new effective techniques should be sought. Among those methods proposed, viscoplastic constant identification of Nafion by employing inverse procedure appears more promising.

An inverse procedure for identifying viscoplastic constants of Nafion utilizes the complex relationship between the FD responses and the material properties. This relationship is often represented by a known mathematical function, which defines the forward problem. Therefore, if a set of reasonably accurate experimental

* Corresponding author. Tel.: +82 32 860 7321.
E-mail address: cdcho@inha.ac.kr (C. Cho).

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FD responses data is available, viscoplastic constants of Nafion may be identified by solving an inverse problem properly formulated. The unknown viscoplastic constants can be determined by minimizing the sum of the squares of the deviations between the experimental FD response data and the calculated one.

The primary objective of this work is, therefore, to develop an effective inverse procedure for identifying viscoplastic constants *A*, *n* and *f* in a two-layer viscoplastic constitutive model of Nafion. Experimental uniaxial tension tests at two different strain rates are conducted to obtain FD response curves. Nafion specimen-specific simulation model is developed and a response surface method [16] is used in conjunction with inverse operator [17] to match experimentally measured and model predicted FD response curves to identify aforementioned unknown viscoplastic material properties.

2. Process for viscoplastic properties identification

2.1. Basic idea

Using the ABAQUS software as a forward problem solver, the FD response of uniaxial tension for polymer Nafion can be obtained using assumed viscoplastic constants *A*, *n* and *f*. Generally, the calculated FD response is different from the experimental one. The inverse procedure can then be formulated by an optimization procedure, which minimizes the sum of squares of deviations between calculated for trail viscoplastic constants and for the actual ones. The transformed optimization problem can be stated as follows:

$$\min_{\mathbf{X}\in\Omega}\left(E(\mathbf{X})=\sqrt{\sum_{i=1}^{N}\left\|y_i^m(\mathbf{X}^t)-y_i^c(\mathbf{X})\right\|^2/N}\right) \tag{1}$$

where $E(\mathbf{X})$ is an assessment function that represents average of least squares error, $\mathbf{X}$ is a unknown constant vector that collects all trail viscoplastic constants *A*, *n* and *f*, y_i^c denotes the calculated FD response using the forward solver, y_i^m is the FD response obtained from uniaxial tension test for actual viscoplastic constant vector $\mathbf{X}^t$, *N* is the number of locations where the FD response is sampled, and Ω is inverse analysis space which covered the possible range of $\mathbf{X}$.

The actual viscoplastic constants $\mathbf{X}^t$ can be inversely identified by solving the optimal problem to minimize the objective function defined in Eq. (1). An effective inverse procedure for this identification problem is outlined in Fig. 1. The procedure mainly consists of experiment, forward calculation and inverse operator, and the detail of each part will be given in the following sections.

2.2. Experiment set up

Nafion 117 was used in all of the uniaxial tension tests. Ten specimens of dog bone shape taken from Nafion 117 were tested on an Instron material testing system at two different initial strain rates (0.01 s^{-1} and 0.001 s^{-1}). Tests were only conducted at room condition, i.e. temperature is 26 °C and relative humidity is 50%, in this work.

For each specimen, the length *l*, width *w* and thickness *t* were measured with a micrometer and a caliper, respectively, at three locations along the specimen before testing. The averages of these measurements *l* = 63.5 mm, *w* = 9.53 mm and *t* = 0.183 mm were used as the nominal dimensions of the specimen. Each specimen was then aligned with the machine axis and clamped in a pair of vise-action grips. The gauge length was adjusted to 30 mm as determined by the grip separation. The average of FD response curve for different strain rates is showed in Fig. 2.

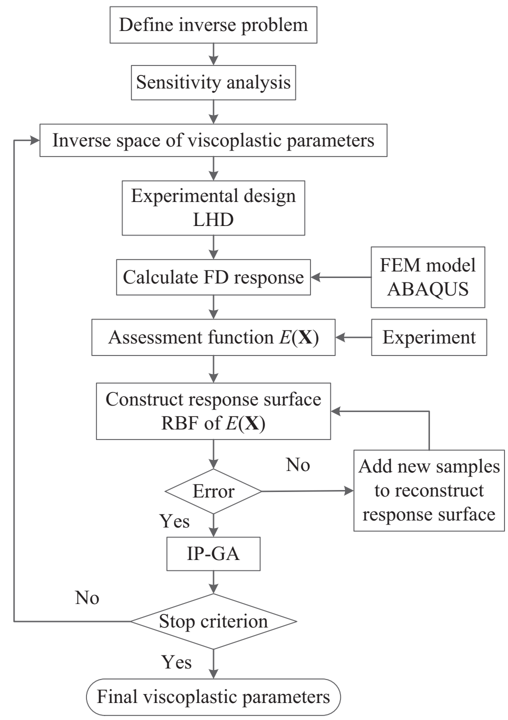

Fig. 1. Flowchart of the present inverse procedure.

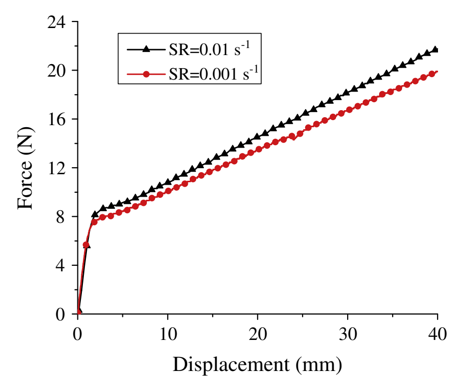

Fig. 2. FD response curves of Nafion at room conditions for two strain rates.

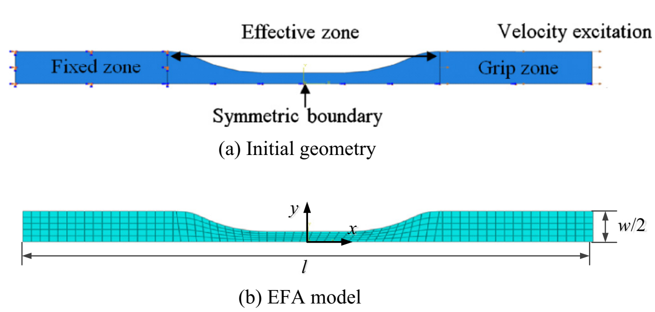

Fig. 3. An (a) initial geometry and (b) specimen specific finite element model.

2.3. Forward calculation

The simulation model for the uniaxial tension event of Nafion is shown in Fig. 3. Due to the symmetric characteristic, only half of the uniaxial tension system is modeled. The model is divided into 265 4-node bilinear plane stress quadrilateral (CPR4) elements in