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MODELLING DIELECTRIC RELAXATION WITH NEURAL NETWORKS

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ABSTRACT. We describe a software model for media with dielectric relaxation. In particular, a model identification is used to measure the phenomenological coefficients which occur in a mathematical description of dielectric relaxation phenomena in electromagnetic media. The identification is developed in order to substitute laboratory dielectric measurements on PMMA and PVC at different frequencies and at fixed temperature so as to obtain the phenomenological coefficients as a function of the frequency.

1. Introduction

In the present work we show that it is possible to obtain an alternative representation of experimental measurements made in laboratory by using the potential of Neural Networks [1, 2, 3]. In particular, we used the model identification to forecast the measure of phenomenological coefficients which occur in the mathematical description formerly proposed by Ciancio in Ref. [4]. With this aim, models for realising a "soft sensor" are implemented, which can supply the behaviour of media with dielectric relaxation. In particular, we considered the behaviour of PMMA (PolyMethylMeta Crylateat) and PVC (PolyVinil Chloride).

2. Dielectric media and phenomenological coefficients

In several previous papers [5, 6, 7, 8, 9, 10, 11, 12, 13, 14] the connection between dielectric and magnetic relaxation phenomena and the occurrence of macroscopic internal degrees of freedom were discussed. Upon introducing a general assumption concerning the entropy, it was shown that the polarization $\mathbf{P}$ can be split in the form

$$\mathbf{P} = \mathbf{P^0} + \mathbf{P^1} \tag{1}$$

where $\mathbf{P^0}$ is the reversible part (elastic) and $\mathbf{P^1}$ is the irreversible part of $\mathbf{P}$, connected with dielectric relaxation phenomena.

Upon neglecting cross effects such as the influence of electric conduction, heat conduction, and mechanical viscosity on electric relaxation, the following differential equation can be derived in the linear approximation [7]:

$$\chi^{(0)}_{(EP)}\mathbf{E} + \frac{\mathbf{dE}}{\mathbf{dt}} = \chi^{(\mathbf{0})}_{(\mathbf{PE})}\mathbf{P} + \chi^{(\mathbf{1})}_{(\mathbf{PE})}\frac{\mathbf{dP}}{\mathbf{dt}} + \chi^{(\mathbf{2})}_{(\mathbf{PE})}\frac{\mathbf{d^2P}}{\mathbf{dt^2}}\,, \tag{2}$$

where $\mathbf{E}$ is the electric field and $\chi^{(0)}_{(EP)}, \chi^{(i)}_{(PE)}$, with $i = 0, 1, 2$, are algebraic functions of the coefficients occurring both in the phenomenological equations and in the equations of state (describing the irreversible processes). The following inequalities hold:

$$\chi^{(0)}_{(EP)} \geq 0\,, \quad \chi^{(i)}_{(PE)} \geq 0\,, \tag{3}$$

$$\chi^{(1)}_{(EP)} - \chi^{(0)}_{(EP)}\chi^{(2)}_{(PE)} \geq 0\,, \tag{4}$$

$$\chi^{(1)}_{(EP)}\chi^{(0)}_{(EP)} - \chi^{(0)}_{(PE)} \geq 0\,, \tag{5}$$

which are connected with stability requirements and with the non-negative character of the entropy production.

3. Identification process and neural networks

In this paper we considered strategies which make direct use of the measurements of the signals produced by the system. This process, called "system identification" allows us to obtain a physical modelling of the system. Different identification strategies by means of input-output measurements are commonly used in many situations in which it is not essential to obtain extensive mathematical knowledge of the system under study but where it is sufficient to predict the evolution of the system. Therefore, the identification approach based on input-output measurements can be applied. A useful approach used for the identification is based on the characterization of the output of the system at a given instant, $y(k)$, by using the following **NARMAX** (Nonlinear Auto-Regressive Moving Average with **eXogenous** inputs) model [15], here reported for **SISO** (Single Input - Single Output) systems:

$$y\,(k) = F\,[y\,(k-1)\,, ..., y\,(k-n_y)\,, u\,(k-1)\,, ..., u\,(k-n_u)] \tag{6}$$

where $y(\dots)$ and $u(\dots)$ are the output and the input respectively at the generic time sample and n_y and n_u are the corresponding numbers of previous samples that it is necessary to consider. A common way to construct a generalized NARMAX model, i.e., valid for different equilibria and even for piecewise linear functions F, is to adopt a "Multi Layer Perceptron Neural Network" which does not need any linearization around equilibria. In fact, whereas the existence conditions of a NARMAX model are valid locally and the function F is assumed to be continuous and differentiable, the approximation of a non linear function F through combination of sigmoid functions, as that performed by a neural network, is effective also for piecewise continuous functions and in wider regions of state space. We used Neural Networks [1, 2, 3] to approximate the F function in Eq. (6). These mathematical models are composed of many non linear computational elements operating in parallel and arranged in patterns that are reminiscent of biological neural nets. Computational elements or nodes are connected via weights that are typically adapted during use to improve performance. The weight of networks represents the parameter to be identified and the learning algorithm, which minimises the quadratic error between the output of the model and the real output of the process, assumes the role of an identification algorithm. In

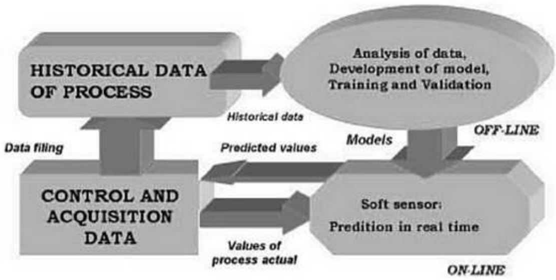

FIGURE 1. Development of a soft sensor

order to exploit the model, it was necessary to determine some parameters. These parameters are the autocorrelation function of the error and the probability density function. The "best conditions" are found when (i) the average error tends towards zero; (ii) the autocorrelation function assumes a trend as similar as possible to a white noise; (iii) the correlation coefficient tends towards one; (iv) the simulated output of the model becomes as similar as possible to the real output of the process. A scheme of the phases of implementation is shown in Fig. 1. We can see that, after the phase of harvest of measures (historical data of the process) in which the aim is to have data representative of operational conditions, the phase of data inspection follows, in which more significant information is obtained through the removal of data related to malfunctions.

4. Models

Many models were realised for PMMA and PVC using neural networks. More specifically, we have used two layers of neurons for each system. The best results, as far as the reliability of the model and the quality indices are concerned, were obtained by increasing the number of neurons. To evaluate all the candidate Neural Networks, we processed experimental data that were provided by the *Istituto per i Processi Chimico Fisici*, a laboratory of the *Consiglio Nazionale delle Ricerche*, and split them into two parts, in order to use one part for the training phase and the other one to test the data according to the scheme illustrated in Fig. 2.

Artificial Neural Networks are based on principles completely different from those typically used for classical artificial intelligence processing. In fact, in a neural network the information is broken down into more elementary information contained within each individual neuron. We can think of a neural network as a system capable of responding to requests and provide an output in response to some input. Each network is divided into layers of neurons; we used a number of layers of neurons ("hidden layers") that is different from input and output ones (see Fig. 3).

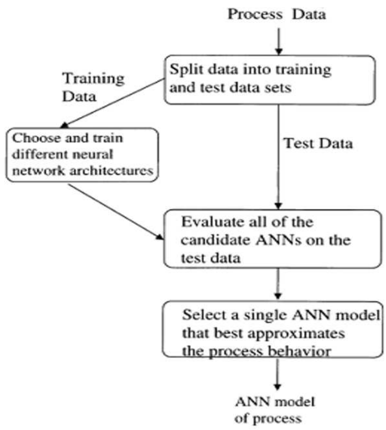

FIGURE 2. Data processing

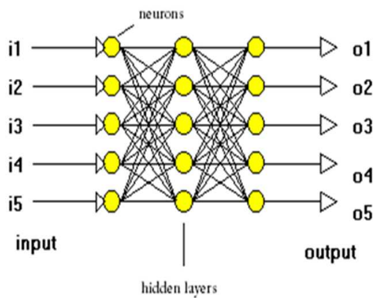

FIGURE 3. Multilayer Neural Network

The transfer function of the network is not programmed, but is achieved through a process of "training" on empirical data. In practice, the network learns the function that links the output with the input through the presentation of examples of real pairs of input and output data; for each input presented to the network in the process of learning, the network provides an output that differs from the correct output: the training algorithm, that was implemented using MATLAB, changes some parameters of the network in the desired direction. Every time an example is presented, the algorithm drives the network parameters towards a set of optimal values for the solution: in this way the algorithm tries to "satisfy" all the examples.

The parameters are the weights and factors linking the neurons that make up the network; in fact, a neural network is composed of a number of neurons connected by links ("weights"), so as to mimic neurons in the human brain. The data on PMMA and PVC were processed using the MATLAB algorithm. We present the results of the best neural networks obtained in the following figures. The plots show that, upon increasing the number of neurons from one to five, the Neural Networks results eventually reproduce the dielectric measurements made in the laboratory.

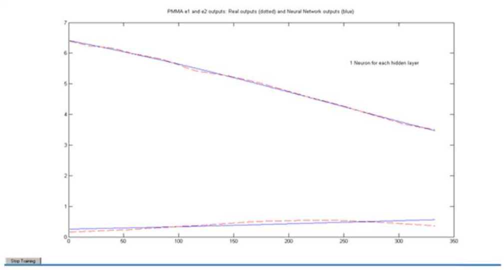

FIGURE 4. PMMA real (dotted) and Neural Network (blue) outputs: one neuron in two hidden layers

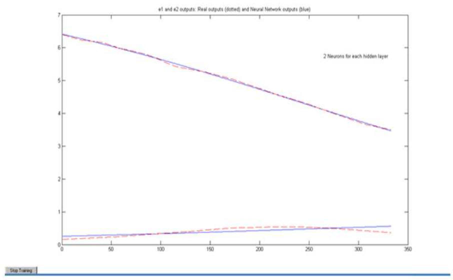

FIGURE 5. PMMA real (dotted) and Neural Network (blue) outputs: two neurons in two hidden layers

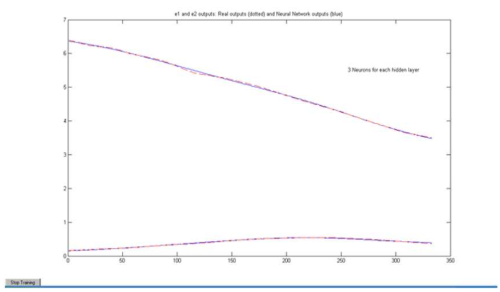

FIGURE 6. PMMA real (dotted) and Neural Network (blue) outputs: three neurons in two hidden layers

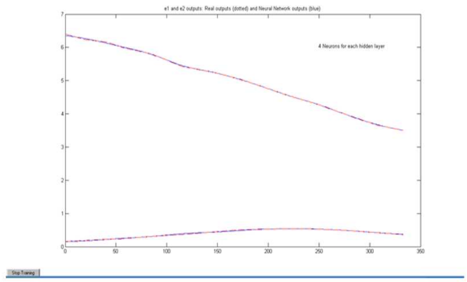

FIGURE 7. PMMA real (dotted) and Neural Network (blue) outputs: four neurons in two hidden layers

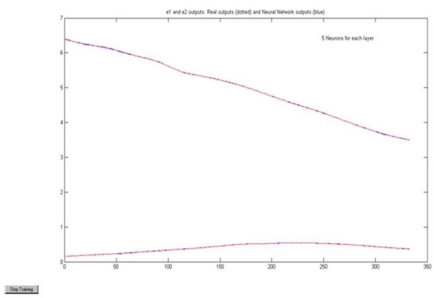

FIGURE 8. PMMA real (dotted) and Neural Network (blue) outputs: five neurons in two hidden layers

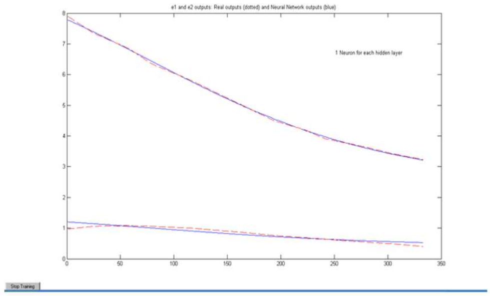

FIGURE 9. PVC real (dotted) and Neural Network (blue) outputs: one neuron in two hidden layers

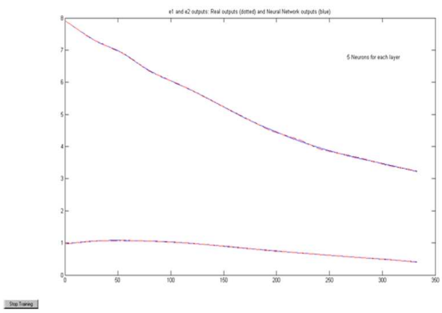

FIGURE 10. PVC real (dotted) and Neural Network (blue) outputs: five neurons in two hidden layers

TABLE 1. Mean square error for Neural Networks with two hidden layers

Neurons	MSE
1	3.6054×10^{-3}
2	3.6048×10^{-3}
3	2.9544×10^{-4}
4	8.7183×10^{-5}
5	6.2244×10^{-5}

5. Conclusions

In this paper we have shown the potential of neural networks in identifying the behavior of PMMA and PVC, with a particular emphasis on the description of dielectric relaxation phenomena in such two media. We verified that, upon increasing the number of neurons in each layer, we reached the best results in terms of quality indices and reliability. Table 1 shows that Neural Networks can mimic the laboratory system with a negligible mean square error (MSE).

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