Creep modelling of Polyolefins using artificial neural networks

M.Nutini, M.Vitali

Basell Polyolefins, a Company of LyondellBasell Industries, Ferrara, Italy

Abstract: Notwithstanding the increasing demand for polymeric materials in an extraordinary variety of applications, the engineers have often only limited tools suitable for the design of parts made of polymers, both in terms of mathematical models and reliable material data, which together constitute the basis for a finite-elements based design.

Within this context, creep modelling constitutes a clear example of the needs for a more refined approach. An accurate prediction of the creep behaviour of polymers would definitely lead to a more refined design and thus to a better performance of the polymeric components. However, a limited number of models is available within the f.e. codes, and when the model complexity increases, it becomes sometimes difficult fitting the models parameters to the experimental data.

In order to predict the polymer creep behaviour, this paper proposes a solution based on artificial neural networks, where the experimental creep curves are used to determine the parameters of a neural network which is then simply implemented in an Abaqus user subroutine.

This allows to avoid the implementation of a complex material law and also the difficulties related to match the experimental data to the model parameters, keeping easily into account the dependence on stress and temperature.

After a discussion of the selection of the appropriate network and its parameters, an example of the application of this approach to polyolefins in a simplified test case is presented.

Keywords: creep, viscoelastivity, polymers, neural networks

1. Introduction

The use of Polyolefins in many aspects of our lives has become so commonplace, that it would be almost impossible to pass a day without coming in contact with a polyolefins-based product. However, despite the increasing use of polymers in engineering products, the stresses and strains that these polymers undergo are often determined as if the behaviour is that of a classical elastic material. Nevertheless, rapid changes are occurring in current engineering practice involving polymers from the perspective of mechanical engineering. Polymers are being considered for increasingly sophisticated industrial applications. The effective and efficient use of these materials requires an understanding of their time-dependent response properties.

The material behaviour of semicrystalline polymers, as polyolefines are, is often characterized as viscoelastic or viscoplastic, which suggests a combination of viscous flow typical for fluids, with either elastic or plastic characteristics typical for solids. The proportion of the viscous, elastic and plastic characteristics depends on the rate of loading, time, loading history, stress level and temperature, and also on the molecular structure.

Most of the approaches available in the literature are material specific, i.e. they are developed for one material, and most of the times they rely on very complex mathematical formulations with several parameters, so that their application to industrial cases is difficult.

In general, constitutive models of polyolefins can be classified either as micromechanical or macromechanical. Micromechanical approaches start with the analysis of the material structure on the molecular level; although extremely useful as a research tool to link the material structure to its mechanical properties, these model however are often not suitable for engineering applications, due to their complexity.

On the other side, for the practical analysis of real structures, macromechanical models can be a better used, these models consisting of some mathematical equations relating strains to stresses at macrostructural levels.

However, the problem using such models is within the approximations and the errors inevitably introduced by the model, as these models are based on simple empirical observations, while the real behaviour of the material is complex. As a consequence, the form taken by the final model may be too specific to generalize beyond new unseen data or too inaccurate to be of use.

What is in fact needed by the engineer is a tool which should be sufficiently simple to be used in the design phase, so that it could easily be interfaced with the most commonly used Finite Element codes for structural analysis; moreover, the tool should be sufficiently general to be applied to a vast class of cases, in terms of materials, load types and loading histories, thus providing a reliable and quick prediction within the accuracy of the state of the art of the finite element analysis.

Within this context, we present a method for determining the creep behaviour of polyolefins which relies on techniques of soft-computing, and in particular incorporates an artificial neural network (ANN) into a creep- subroutine to be used with Abaqus/Standard for structural analysis, in an efficient and very simple way.

Neural networks are increasingly used as alternatives to mathematical constitutive modelling. The approach using ANN relies on the capabilities of the neuron model to learn the non-linear relationship between input and output parameter in the system.

In the literature, a restricted number of examples of the application of ANN-based techniques to model constitutive laws is available (e.g. Furukawa, 1998; Sen, 2002; Reithofer, 2007) In particular, a neurocomputational viscoplastic model was proposed by Al-Haik et al. (Al-Haik, 2003), where an artificial neural network is used to determine the creep behaviour of a composite. In particular, an ANN is used to predict the creep strain when the stress, the time and the temperature are provided in input. The work of Al-Haik is also focused on the evaluation of different algorithms for training the network, and a new second-order algorithm for training a multilayered neural network is presented.

The present paper uses an approach similar to that of Al-Halik; however, due to the needs for interfacing with a Finite Element code, to be used in the design of industrial components having even millions of element, a simpler network topology is sought, aiming to reduce the computational times; this will result in a different selection of the training data set, showing that for the application presented the ANN can be better trained to predict the creep strain rate rather than the creep strain.

Finally, after some considerations based on a rough finite element reproduction of the creep test used to derive the material data, a simple benchmark test is presented for the validation of the approach.

2 Artificial Neural Networks

In this paragraph the fundamentals of Artificial Neural Networks theory and application are briefly reviewed (Zio, 2007)

Neural networks are information processing systems composed of simple processing elements (nodes) linked by weighted connections (Eberhart, 1990). Here we limit ourselves to describing the most commonly used multi-layered feed-forward neural network which, in its simplest form, consists of three layers of processing elements: the input, the hidden and the output layers, with ni, nh and no nodes respectively (Fig. 1).

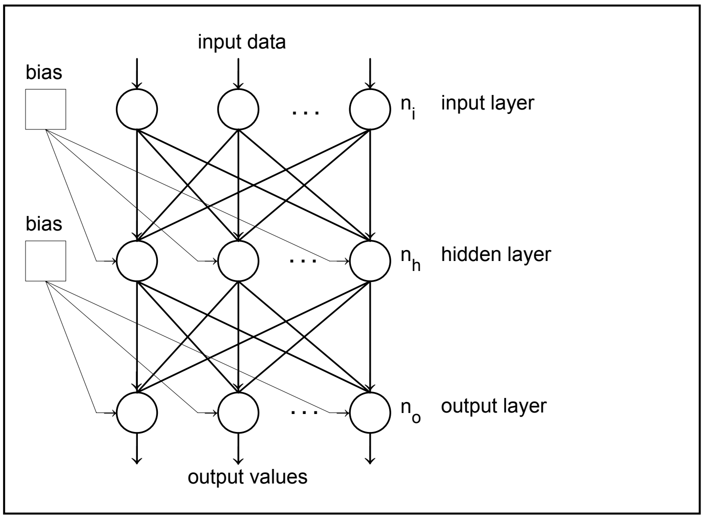

Figure 1. Scheme of a three-layered, feedforward neural network.

The signal is processed forward from the input to the output layer. Each node collects the output values, weighted by the connection weights, from all the nodes of the preceding layer, processes this information through a sigmoidal function

$$f(x) = 2\,(1 + e^{-x})^{-1} + 1$$

and then delivers the result towards all the nodes of the successive layer. The sigmoidal function used in this work is represented in fig. 2.

In the present work both input and hidden layers have the additional bias node, which is often employed as a threshold in the argument of the activation function and whose output always equals unity.

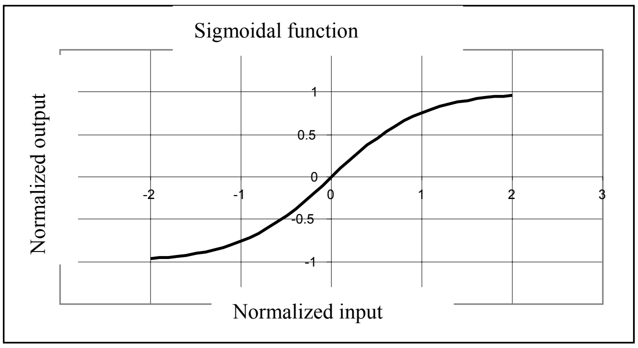

Figure 2. Sigmoidal function used.

The values of the connection weights are determined through a training procedure. In this case we have adopted the usual error back-propagation algorithm which follows from the general gradient descent method. In short, the back-propagation algorithm performs the steepest descent in the weight space on a surface, whose height at any point is equal to the error function. It consists of an iterative gradient algorithm designed to minimize the mean square error between the actual network output and the true value. Sets of np input and associated no outputs are repeatedly presented to the network and the values of the connection weights are modified so as to minimize the average squared output deviation error function, or Energy function, defined as

$$D = \frac{1}{2n_p n_o} \sum_{p=1}^{n_p} \sum_{l=1}^{n_o} (t_{pl} - o_{pl})^2$$

where t_{pl} and o_{pl} are the true and the network-computed values of the l-th output node, to the p-th pattern presented. Through this training procedure, the network is able to build an internal representation of the input/output mapping of the problem under investigation. The success of the training strongly depends on the normalization of the data and on the choice of the training parameters. In this work, each signal has been transformed by an affine mapping in the interval (-1, +1); the learning coefficient and the momentum factor are 0.05 and 0.9, respectively; moreover the connection weights have been initialized randomly. After the training is completed, the final connection weights are kept fixed. New input patterns are presented to the network which is capable of recalling the information stored in the connection weights during training to produce the corresponding output, coherent with the internal representation of the input/output mapping. This is called the “recall” phase.

Notice that the non-linearity of the sigmoidal function of the processing elements allows the neural network to learn arbitrary nonlinear mappings. Moreover, each node acts independently of all the others and its functioning relies only on the local information provided through the adjoining connections. In other words, the functioning of one node does not depend on the states of those other nodes to which it is not connected. This allows for efficient distributed representation and parallel processing, and for an intrinsic fault-tolerance and generalization capability.

These attributes render the artificial neural networks a powerful tool for signal processing, nonlinear mappings and near-optimal solution to combinatorial optimization problems.

For the present paper the Matlab Neural Network Toolbox (Demuth, 2004), which implements all the features described above, has been used.

3. Creep testing

The measurement of creep data on polypropylene samples used for the present paper, carried out at at Basell laboratories in Ferrara, is based on a three points bending test. This method is the same used at Basell to generate data for CAE simulations for its internal use and according to the requests from the customers. The same methodology has been maintained for this work, as the purpose of the whole activity is to set a procedure and a technique which could be easily implemented and adjusted in a routine practise and in an industrial environment. Accordingly, this paragraph describes also a standard testing procedure followed at Basell.

The specimens are cut from injection moulded plaques - having dimensions 150 mm x 250 mm, with a thickness of about 3.2 mm.- transverse with respect to the injection flow. The specimens are cut in shape of rectangles, having a with of 12.7 mm and a length of 90 mm. For testing at low stresses, as per example at less than 1 MPa, specimen having a width of 25 mm have been used. The test is done in a conditioned oven, with preconditioning of at least one hour at the test temperature. For each temperature usually four levels of stress are tested, usually up to around the 70% of the maximum stress measured in the static tensile test at the same temperature. The duration of the test is usually 22 hours or 1 week, but for the samples used for the present work only 22 hours tests have been carried out. For the detailed description of the test, reference is made to fig. 3. The specimen **1** lays on two supports **2**, whose span is 60 mm., having a rounded contacting surface **3**. The load is applied by placing onto the mid of the specimen, equally spaced from the supports, an aluminium cylinder **4**, having a diameter of 10 mm, which extends through the whole width of the specimen, to which appropriate weight are suspended through the wires **5**. A thin rod **6** is let to lay onto the surface of the cylinder **4.** The rod **6** is connected at its upper extremity to a gauge **7** for measuring the displacement. The whole assembly is fitted in an oven, although the rod **6** is long enough to allow locating the gauge **7** outside of the oven itself, to which it is fixed.

For the measurement a gauge Marposs is used with an accuracy of 0.001 mm, communicating through the serial port to a PC, which records and stores the displacement values.

Different weights can be selected in order to apply the desired load. In order to generate a prescribed level of stress, the value of the weight to be applied is calculated using an approximate formula for three points bending for small strains (Roark, 1954).

During the initial part of the transient, after the load application, the signal from the gauge is stored every second.; thereafter the acquisition interval is gradually increased, up to an interval of 4 hours at the end of a 22 hours total acquisition time.

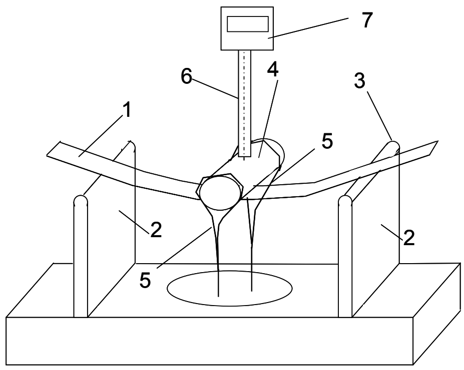

Figure 3. Experimental layout for a three points bending test.

4. Network selection

A first concern in the selection of the network topology was to limit the number of hidden nodes. In fact, this helps in reducing the computational effort when using the ANN to predict the creep strain during the structural analysis. As this is supposed to occur for each element and for each iteration, limiting the operations carried out by the networks definitely helps in saving CPU times during the finite element simulation. Moreover, an ANN with too many hidden nodes learns the training set data *by heart*, but it fails in the recall phase, i.e. it has not generalization capability. Additionally, in the present work ANN having one hidden layer only have been employed, as it has been shown that these networks are "Universal Approximants", i.e. they are suitable to approximate any function with its derivatives with a desired level of accuracy. (Hornick, 1990; White, 1990)
Accordingly, a first network with two input nodes, one hidden layer with two nodes and one output layer having one node only was the primary choice. The number of nodes in the input nodes generally corresponds to the number of variables from which the requested prediction is supposed to depend. The number of nodes in the output layer reflects instead the variables to be predicted. It was reasonably chosen to provide in input the time and the stress, thus expecting the network to predict the strain.
With this approach the results were disappointing. An example is reported in fig. 4, relative to a talc-filled Polypropylene elastomer modified. In this case the training set comprised data measured at 80°C at 0.5, 1., 1.2, 1.7 and 2 MPa., with times ranging from 0 to 1320 minuts, for a total number of 503 patterns randomly distributed

When the training input data were proposed to the network, the response was apparently satisfactory, as visible from the general trend in fig. 4 (left). However, some discrepancies are visible for the very initial part of the transient (as per fig. 4, right)

For a preliminary validation of the network, a simplified finite element simulation of the creep test itself was executed, as a sort of “reverse problem”, using Abaqus/standard, version 6.7. This finite element analysis models the specimen as a rectangle 12.7 mm x 90 mm, where the nodes laying on the median section are subjected to a point load, simulating the weight applied with cylinder 4 of fig.3. Symmetrically with respect to this central raw of nodes,, at a distance there from of 30 mm, two rows of nodes are fixed in Z, thus simulating the supports 3 of fig. 3.

A number of 2000 S4-R elements having a thickness of 3 mm., shaped as squares of about 3 mm size have been used.

The maximum specimen deflection obtained with the ANN prediction of the strain is represented by the dashed line in fig. 5. It is believed that the scarce accuracy of the network in the prediction of the initial part of the transient causes the consequent inaccurate prediction of the deflection in the remaining part of the transient, beyond the unavoidable errors due to the extreme simplification of the analysis.

Accordingly, some trials were executed by introducing several ANN, each devoted to reproduce a specified part of the transient in the space stress/ time. However, the experience posed severe problems of convergence, so that an alternative approach has been introduced.

Based on the needs for an accurate prediction of the strain rate, and also in agreement to some indications available in the Abaqus User Manual (Abaqus, 2007) about writing a user subroutine for CREEP modelling, the authors here propose a method by which an ANN is used to predict the creep strain rate $\dot{\varepsilon}$, there from evaluating the creep strain increment as $\Delta\,\varepsilon = \dot{\varepsilon}\,\Delta t$, Δt being the time increment in the finite elements analysis.

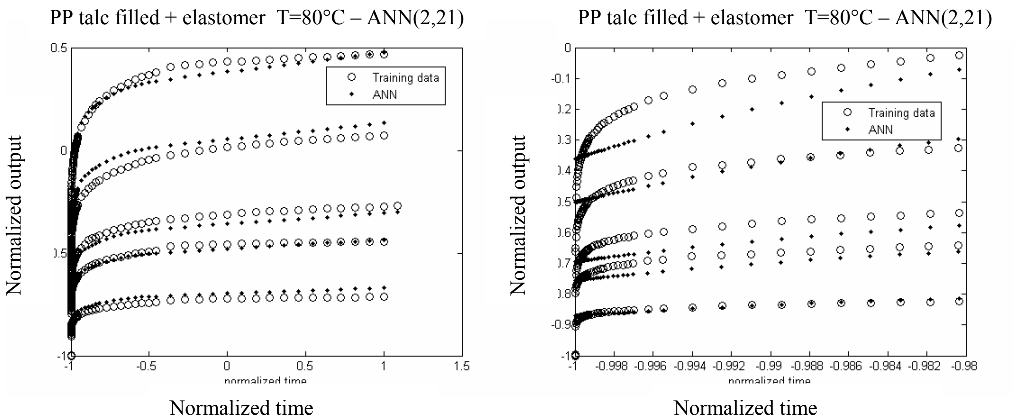

Figure 4. Talc filled+elastomer PP, T=80°C ANN trained to reproduce the strain.

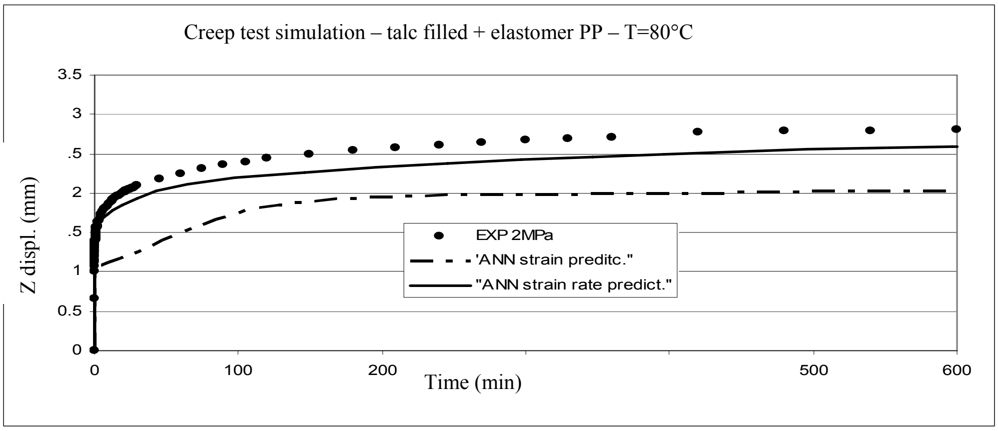

Figure 5. Results on the creep test reproduction through F.E.

For this class of materials, during the creep test the strain rate can vary of some orders of magnitude. An example is computed for the talc filled+elastomer PP discussed above, where the strain rate has been used derivating the piecewise 4th order polynomial interpolation of the strain vs. time curve. Due to its rapid variation and the enormous data range, it has been preferred to train the network on the logarithm of the strain rate (with sign changed). An example of the values computed for such material is in fig. 6.

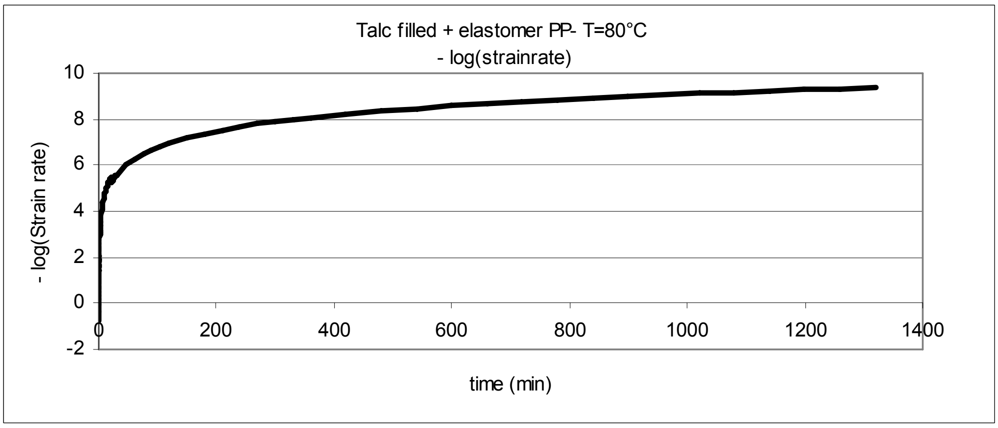

Figure 6. logarithm of theStrain rate (sign changed) measured during the creep test, example: (talc filled – elastomer charged PP, T=80°C, 6MPa)

Accordingly, a (2,2,1) ANN (2 nodes in the input-, 2 nodes in the hidden- and 1 node in the output-layer) has been trained using the stress and the time as input and the logarithm of the strain rate as output. A number of 396 patterns was proposed to the network, comprising data measured at 0.5, 1, 1.7 and 2 MPa. At 80°C. The data at 1.2 Mpa were not used in the training.

The response of the network on the training data set is quite acceptable (fig. 7), as also the response of the network when the data at 1.2 MPa were used to test the network (fig. 8)

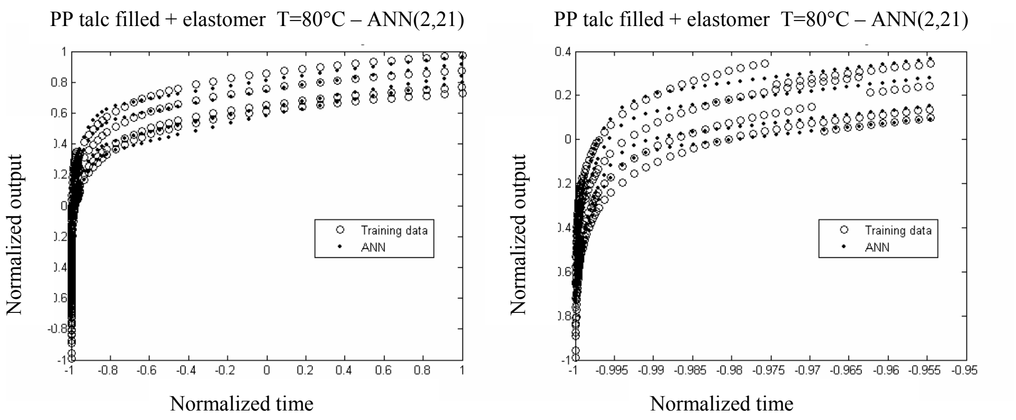

Figure 7. Talc filled + elastomer PP, T=80°C ANN prediction on training data – output: logarithm of the strain rate (sign changed)

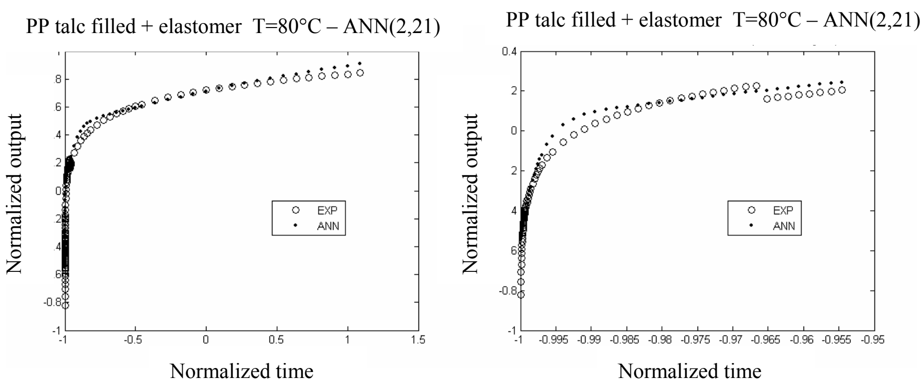

Figure 8. Talc filled + elastomer PP, T=80°C ANN prediction on data (output: log. of the strain rate- changed sign) not in the training set

Discontinuities in the first derivative of the training data are accepted and smoothened by the network.

The ANN obtained is used in the finite element reproduction of the creep test. The predicted maximum deflection of the specimen, represented in fig. 5 by the continuous line, is in good agreement – within the accuracy of the model – with the experimental data. To better validate this approach, a dedicated benchmark test is presented in the following paragraph.

5. Validation test: experimental set-up

A benchmark test has been set up at Basell (Bonaldo, 2007) to validate computational models and material data. In particular, the test is suitable for the validation of creep data.

The test is carried out on an injection moulded plaque having dimensions 150 mm x 300 mm and a thickness of about 3 mm. As shown on fig.9, the plaque is fixed at three corners to an aluminium frame through bolts; both plaque and frame are inserted into an oven, so that the temperature is controlled. The frame is supported by aluminium screws, which allow the operator to accurately level the frame and the plaque as well. A light vertical carbon rod is supported at its low extremity by the plaque itself, while at its upper extremity it is connected to a gauge for displacement measurement. The gauge is fixed onto the structure of the oven, so that the only load insisting on the plaque due to the gauge is that caused by its internal spring.

The weight exerted by the rod and by the gauge has been totally measured as 50 g, averaged through the spring elongation. The location of the point where the rod touches the plaque (measuring point) is in proximity of its free corner.

In the first test ("Test No. 1"), an additional 500g load is suspended at the plaque from the measuring point through a hook fixed to the plaque itself. A second test ("Test No. 2") is carried out in order to onset a different stress distribution, to evaluate the network capability of accurate predictions in a different range of stress values. In this case a 500 g weight is suspended from the plaque through a hook fixed at about 140 mm from the measuring point. The location of of the points on the plaque where the load is applied is schematically represented in fig.9.

In both the tests the material used is a talc filled polypropylene.. Both the tests have been executed at 23°C for an overall duration of 8 hours.

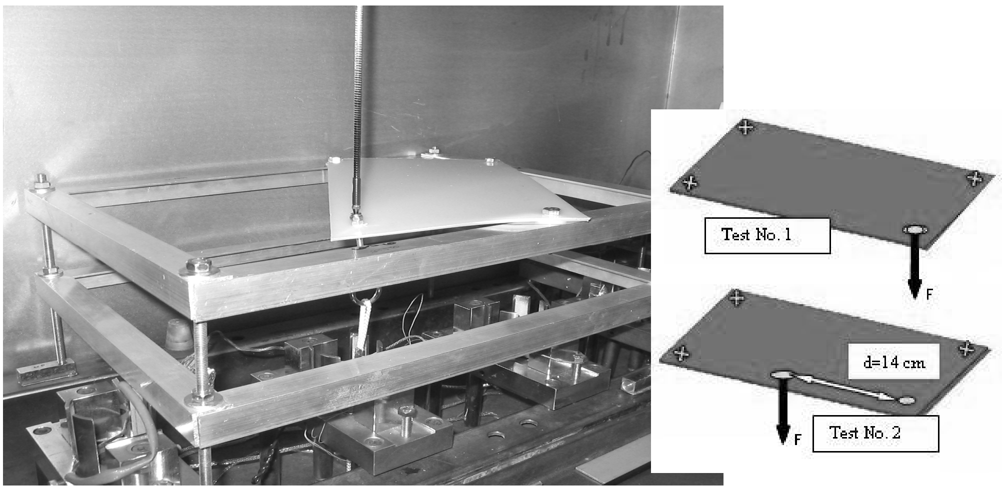

Fig. 9. Validation test – Experimental set-up.

6. Finite Element Reproduction of the Validation test

The validation test has been simulated through Abaqus/standard Version 6.7, with a CREEP user subroutine incorporating the Neural Network obtained from the training. In a first case, a talc-filled material plaque has been subjected to the test with a 500 g. load applied at the hook located under the measuring point.

For the simulation a mesh with square S4R elements with the size of about 4 mm. has been used, with local refinement in proximity of the fixing. The stress-strain data used to simulate the static loading were derived from a tensile test. In this case. the specimens, shaped according to the standard ISO R527, were cut from a injection moulded plaque with the dimensions as the plaques used for the validation test. As the polymer used is anisotropic, two sets of data were obtained, using specimens cut at different orientations (transverse and longitudinal) with respect to the injection flow. Correspondingly, two simulations were carried out, with transverse and average data respectively.

For this test case a (2,2,1) ANN has been trained on experimental creep data taken 1,4,6 and 10 MPa. The input provided to the networks were the stress and the time, nornalized in the interval 2 to 10 MPa and 0 to 1320 hours. The output of the net is the natural logarithm of the strain , normalized between 1and 11 The values have been mapped into an interval -1 – 1. The sigmoidal activation functions was used for the input and the hidden layer, while a linear function has been used for the output layer. The adopted learning rate was 0.03, the momentum was 0.9

The network obtained is definitely capable of reproducing the input data, as shown in fig. 10. Here one can also notice that the training data show a certain degree of irregularity. This is caused by the piecewise polynomial interpolation used on the raw strain data to derive the strain rate data, as the interpolation was not ensuring continuity of the first derivative. However, the network itself compensates for this interpolation error; consequently, the curves predicted by the ANN are smooth.

The load to be applied for this test case has been chosen in order to onset a stress distribution on the plaque with values in the range of the training data.

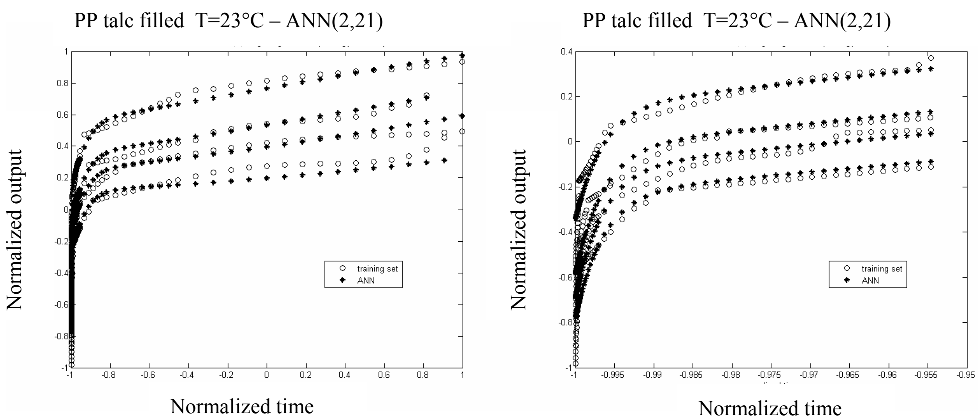

Fig. 10. Test No. 1: ANN prediction on training data (left); and detail (right)

In fact, the stress distribution obtained at the end of the static load is characterized by a significant portion of the computational domain having Von Mises stresses from 1 to 2 MPa, with peaks of about 4.5 MPa in proximity of the fixings (fig. 11, result with average material tensile data). For stresses lower than the smallest stress used in the training , the creep strain was computed by simply proportionally scaling the strain predicted by the ANN for the lowest training data stress.

At the end of the creep phase, whose duration is 8 (eight) hours, the displacement field obtained is depicted in fig. 12.

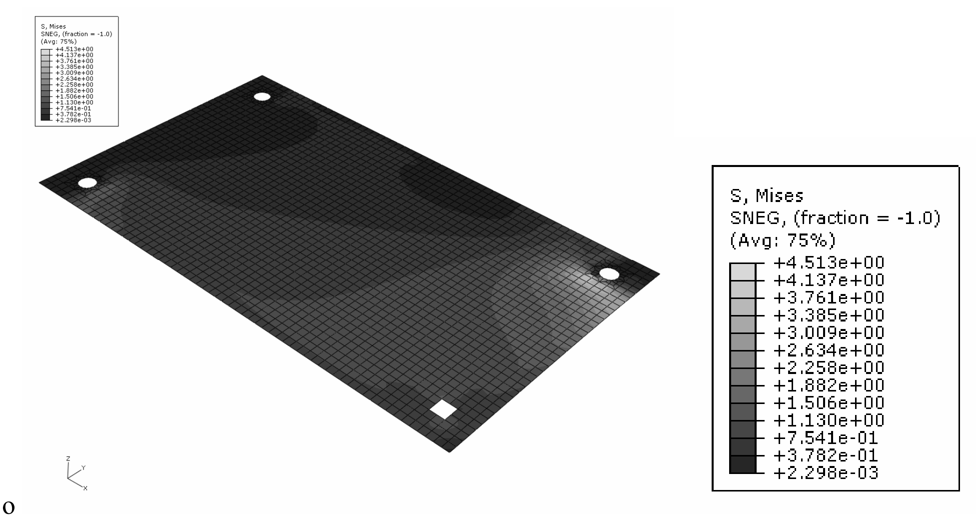

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Fig. 11. Test No. 1-. Von Mises stress distribution

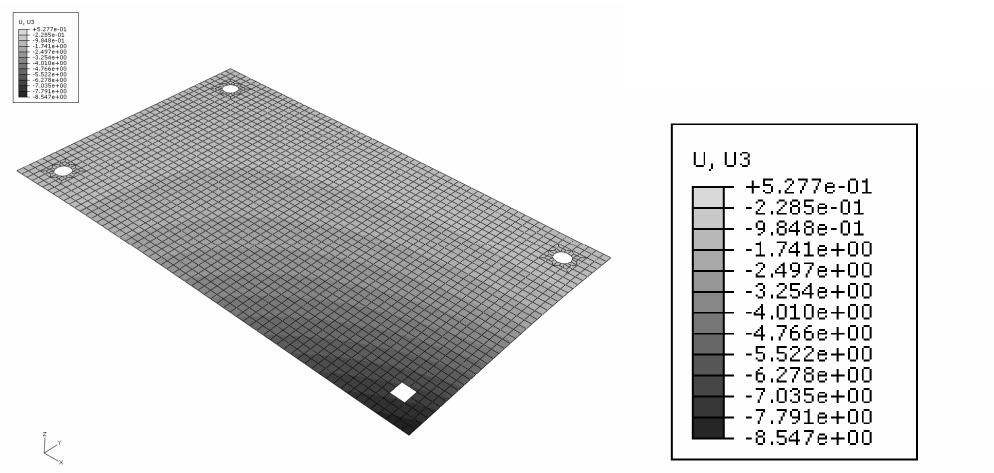

Fig. 12. Test No. 1 - Z displacement distribution

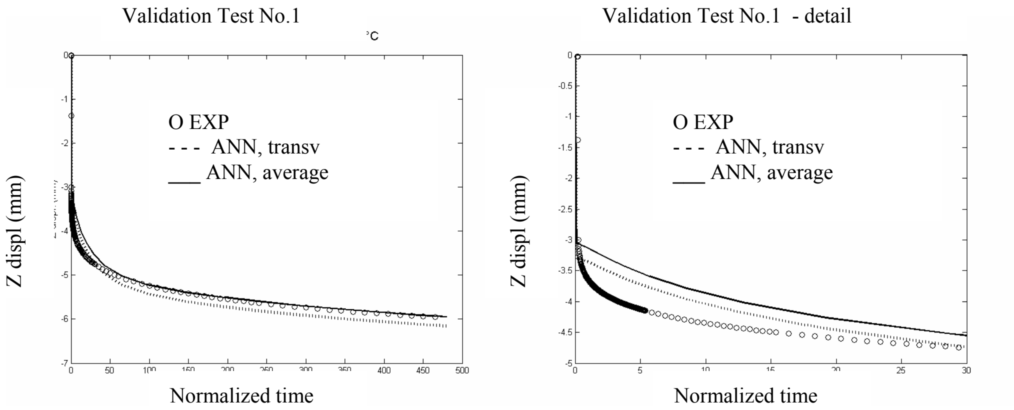

Fig. 13. Test 1. - Displacement of the measurement point - Comparison between F.E. analysis and Experiment.

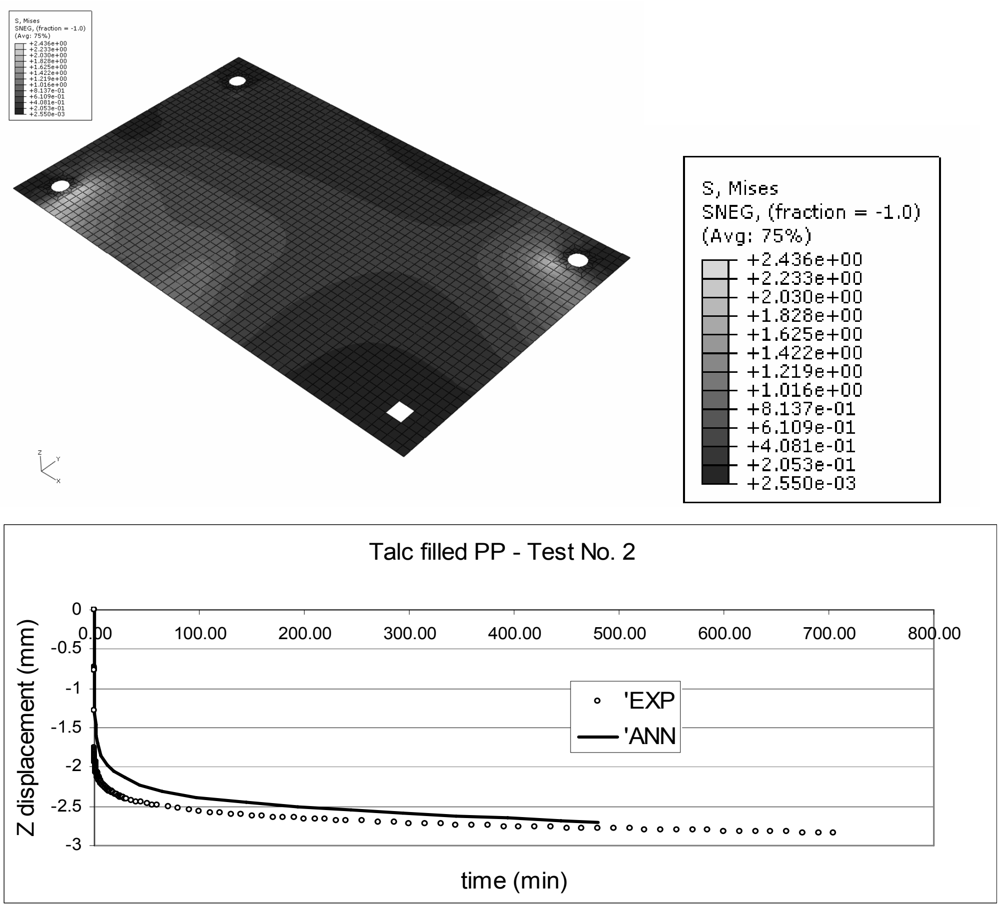

Fig. 14. Test No. 2-. Von Mises stress distribution (above); Z displacement: comparison with the experimental measurement (below)

The displacement evolution computed for the node corresponding to the measurement point is compared to the values recorded by the gauge in fig. 13 (left). Two curves from F.E. analysis are reported, corresponding to the two sets of tensile test data available, in order to see the effect of the material anisotropy.

In both the cases the ANN-based creep routine well predicts the creep evolution. Apart from the very first initial transient after the load application (fig. 13, right), the general agreement of the F.E: simulation with the experimental value is definitely quite acceptable

The same approach has been used for the "Test No. 2". The stress distribution obtained at the end of the static loading is reported in fig. 14 (left). The comparison between the displacement measured and the one computed is displayed in fig. 14 as well (right).

7. Conclusions

The use of artificial neural networks, implemented in a user subroutine for Abaqus/Standard, to predict the creep behavior of polymers in a structural analysis has been presented, with satisfactory results.

The approach has been validated using an experimental dedicated benchmark test, which has been designed and developed at Basell laboratories in Ferrara.

Considering the accuracy of the predictions obtained with this method, it can be stated that the artificial neural networks have been proved to be a practical and efficient tool for simulating the viscoelastic behavior of polyolefins in a structural analysis; moreover, they can be easily and efficiently implemented and interfaced with Abaqus/ standard.

8. References

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