MODELING OF REACTIVE POLYMER COMPOSITE MOLDING PROCESSES USING NEURAL NETWORKS

JIE ZHANG[1], Nikos G. Pantelelis[2]
[1]School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle upon Tyne NE1 7RU, UK, e-mail: *jie.zhang@newcastle.ac.uk*
[2]Mechanical Engineering Department, National Technical University of Athens, Greece

SUMMARY

This paper presents a self-learning method for the real-time calculation of the degree of cure and Tg in polymer composite molding using bootstrap aggregated neural networks based and recordedprocessing data such as the temperature and the electrical resistance of the resin. In order to improve model generalization capability, multiple neural networks are developed from bootstrap re-samples of the original data and are combined. The proposed method is successfully applied to real industrial data.

1. INTRODUCTION

Polymer composite materials have been increasingly used in many areas, for example, aerospace, automobile, and construction industries, due to their various advantages (1). The degree of cure and glass transition temperature are important parameter in reactive polymer composite molding processes. Only when the product is almost fully cured and the required glass transition temperature is reached the mould can be opened. Thus, modeling the degree of cure is very important in the control and optimization of reactive polymer composite molding processes. Development of detailed mechanistic models for the degree of cure is generally time consuming and effort demanding. Data based empirical modeling can be a very useful alternative in this case. Neural networks have been shown to be capable of approximating any continuous nonlinear functions (2) and have been applied to nonlinear process modeling (3, 4).

A problem of conventional neural network is the lack of robustness and generalization capability due to limitation in training data and/or training methods. An effective approach to improve neural network model generalization is by combining multiple neural networks (5, 6, 7). The paper presents a study on using bootstrap aggregated neural networks for modeling the degree of cure and glass transition temperature of an industrial reactive polymer composite molding process.

2. MODELLING OF REACTIVE POLYMER COMPOSITE MOLDING PROCESS USING NEURAL NETWORKS

2.1 Bootstrap Aggregated Neural Networks

A diagram of bootstrap aggregated neural networks is shown in Fig. 1, where several neural network models are developed to model the same relationship. Instead of selecting a “best” single neural network model, these individual neural networks are combined together to improve model accuracy and robustness. The overall output of the aggregated neural network is a weighted combination of the individual neural network outputs. This can be represented by the following equation.

$$f(X) = \sum_{i=1}^{n} w_i f_i(X) \quad (1)$$

where $f(X)$ is the aggregated neural network predictor, $f_i(X)$ is the ith neural network, w_i is the aggregating weight for combining the ith neural network, n is the number of neural networks, and X is a vector of neural network inputs. The aggregating weights can be obtained using a number of ways, such as simple averaging, i.e. the stacked neural network output is an average of the individual network outputs, or using principal component regression (PCR) (7). Instead of using constant stacking weights, the stacking weights can also dynamically change with the model inputs (8, 9). Another advantage of bootstrap aggregated neural network is that model prediction confidence bounds can be calculated from individual network predictions (10).

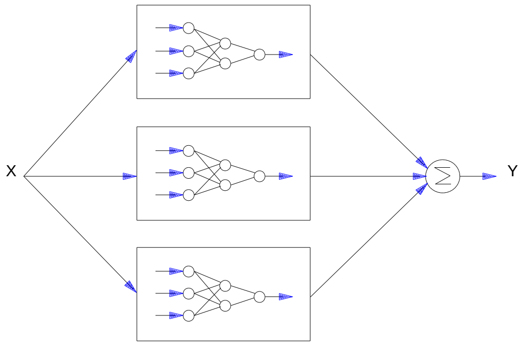

Figure 1. A bootstrap aggregated neural network

2.2 Modeling the Degree of Cure in an Industrial Polymer Composite Molding Process

Neural network models were developed using industrial data from an EU research project – iREMO (intelligent reactive polymer composite molding). The process is for the manufacturing of automobile parts. The molding process is monitored using OptiMould which measures resistance. Data from 3 days of process operation during June 2011 were used to build and validate the neural network models. The data set contains 94 runs where constant curing temperature policy was applied. Variations in mould temperature exist due to exothermal effect. Data from 15 runs were selected as the model building data, which were randomly split into training set (50%) and testing set (50%). The final developed model was tested on all other runs.

The developed neural network based dynamic model is of the following form:

$$logR(t)=f(logR(t\text{-}1),\ logR(t\text{-}2),T) \tag{2}$$

where R is the resistance, T is the average temperature during the first 4 minutes, t is discrete time, $f()$ is a nonlinear function represented by the neural network.

A bootstrap aggregated neural network containing 30 single hidden layer neural networks was developed. The number of hidden neurons in each network was determined through cross validation. The networks were trained with Levenberg-Marquardt algorithm with regularization and early stopping. Figure 2 shows the predicted resistance on 4 selected unseen validation runs. In Figure 2, the actual measured resistances are shown as the solid lines, one-step-ahead predictions are shown as dash-dotted lines, and multi-step-ahead predictions are shown as the dashed lines. It can be seen that the neural network one-step-ahead predictions are very accurate. The multi-step-ahead predictions are also very accurate, though not as accurate as the one-step-ahead predictions.

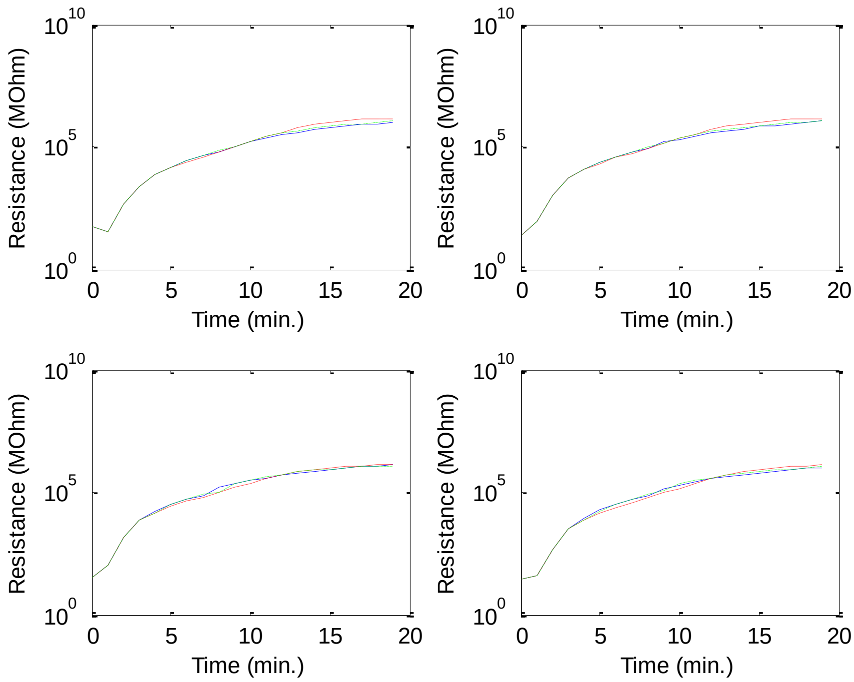

Figure 2. Dynamic neural network model predicted resistance on 4 unseen runs

As the ultimate interests in monitoring and control of reactive polymer composite molding processes are concerned with the degree of cure and the glass transition temperature (T_g), it would be desirable that the neural network predicted resistance is converted into the degree of cure and the glass transition temperature. The assumption made here is that the changes in the measured resistance reflect the changes in the degree of cure and T_g, which is the principle that OptiMould is based on.

For a given molding temperature, the maximum degree of cure can be calculated using Eq(3) obtained by studies carried out within the iREMO project.

$$\alpha_{\max} = 0.409 + 0.00145T \qquad (3)$$

where T is the molding temperature and $\alpha_{\max}$ is the maximum degree of cure under this molding temperature.

Let the minimum and maximum predicted resistances in a curing cycle correspond to the minimum and maximum degrees of cure respectively, then the estimated degree of cure for a given predicted resistance can be obtained as:

$$\alpha = \frac{\log \hat{R} - \log \hat{R}_{\min}}{\log \hat{R}_{\max} - \log \hat{R}_{\min}} \alpha_{\max} \qquad (4)$$

where $\hat{R}$ is the neural network model predicted resistance, $\hat{R}_{\min}$ and $\hat{R}_{\max}$ are the minimum and maximum predicted resistance respectively, and $\alpha_{\max}$ is the maximum degree of cure.

From the estimated or predicted degree of cure, glass transition temperature can be obtained. The relationship between the degree of cure and the glass transition temperature is given by Eq(5).

$$\frac{T_g - T_{g0}}{T_{g\infty} - T_{g0}} = \frac{\lambda\alpha}{1-(1-\lambda)\alpha} \qquad (5)$$

where T_g is the glass transition temperature, α is the degree of cure, λ = 0.44, T_{g0} = 241 K, and $T_{g\infty}$ = 427 K. By re-arranging Eq(5), the following equation for predicting glass transition temperature is obtained.

$$T_g = T_{g0} + \frac{\lambda\alpha(T_{g\infty} - T_{g0})}{1-(1-\lambda)\alpha} \qquad (6)$$

Neural network predictions of degree of cure and glass transition temperature from the neural network model on the unseen validation data are obtained using the predicted resistance shown in Figure 2, Eq(4), and Eq(6). Figure 3 shows the predicted degree of cure while Figure 4 shows the predicted T_g. In both figures, the actual values converted from the measured resistances are shown as the solid lines, one-step-ahead predictions are shown as dash-dotted lines, and multi-step-ahead predictions are shown as the dashed lines. It can be seen from Figures 3 and 4 that the predictions are very accurate.

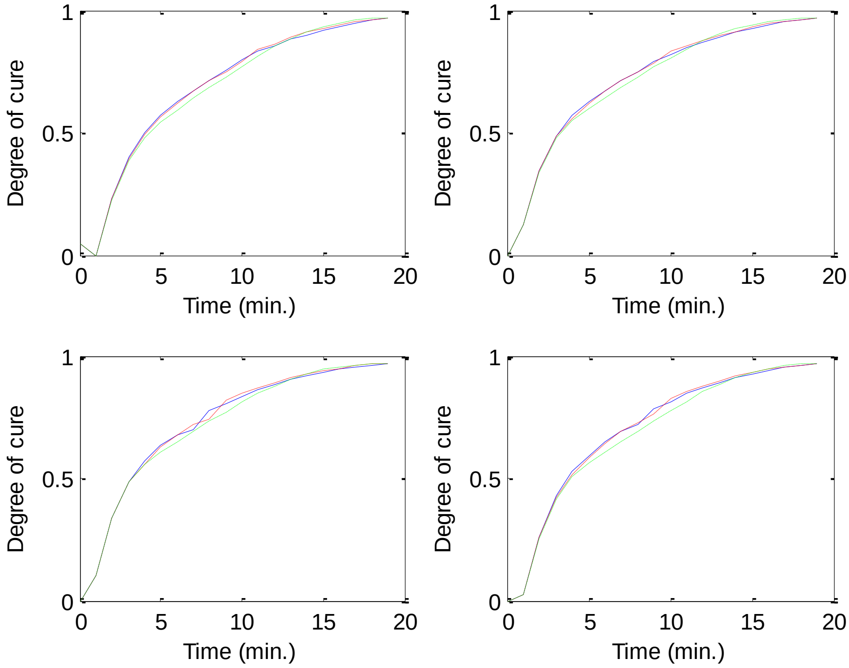

Figure 3. Dynamic neural network model predicted degree of cure on 4 unseen runs

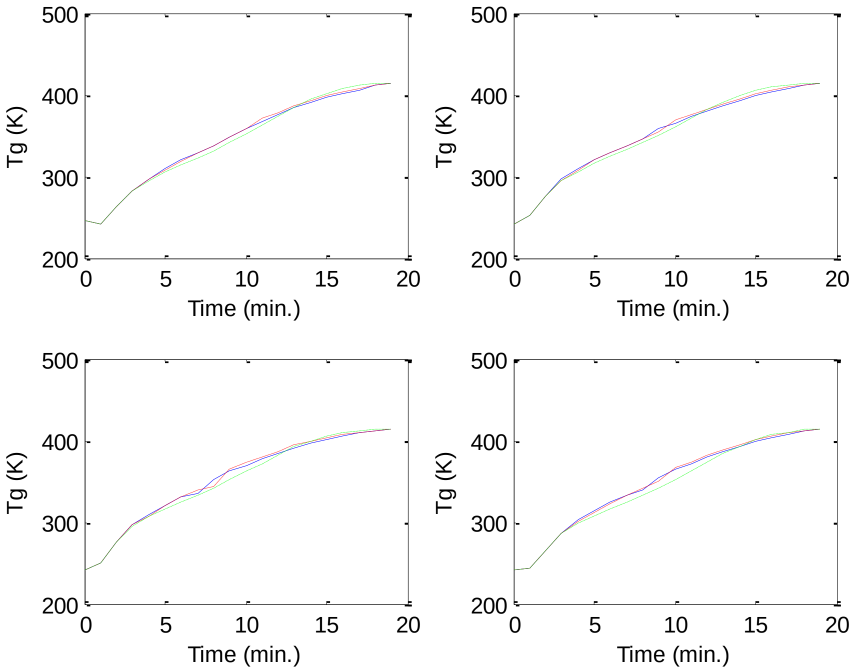

Figure 4. Dynamic neural network model predicted T_g on 4 unseen runs

4. Conclusions

Modeling of an industrial reactive polymer composite molding process using bootstrap aggregated neural networks is presented in this paper. By combining multiple neural network models, model prediction accuracy and reliability are improved. Application results demonstrate that the developed neural network models can accurately predict the degree of cure and glass transition temperature. The developed neural network model can be used for calculating the optimal heating profile, determining when the mould can be opened, and product quality monitoring.

Acknowledgement

The research is supported by the EU through the project iREMO – intelligent reactive polymer composite molding (contract No. NMP2-SL-2009-228662).

REFERENCES

1. N. G. Pantelelis, "Towards the dynamic optimisation for the cure control of thermoset-matrix composite materials", Composites Science and Technology, 65 (2005) 1254–1263.
2. G. Cybenko, "Approximation by superposition of a sigmoidal function", Math. Control Signal Systems, 2 (1989) 303-314.
3. N. V. Bhat, and T. J. McAvoy, "Use of neural nets for dynamical modelling and control of chemical process systems", Computers & Chemical Engineering, 14 (1990) 573-583.
4. A. B. Bulsari (Ed), Computer-Aided Chemical Engineering, Vol.6, Neural Networks for Chemical Engineers, Elsevier: Amsterdam, (1995).
5. L. Breiman, "Bagging predictor", Machine Learning, 24 (1996) 123-140.
6. D. V. Sridhar, R. C. Seagrave, and E. B. Bartlett, "Process modelling using stacked neural networks", AIChE Journal, 42 (1996) 2529-2539.
7. J. Zhang, A. J. Morris, E. B. Martin, and C. Kiparissides, "Inferential estimation of polymer quality using stacked neural networks", Computers & Chemical Engineering, 21 (1997) s1025-s1030.
8. Z. Ahmad and J. Zhang, "Bayesian selective combination of multiple neural networks for improving long range predictions in nonlinear process modelling", Neural Computing & Applications, 14 (2005) 78-87.
9. Z. Ahmad and J. Zhang "Combination of multiple neural networks using data fusion techniques for enhanced nonlinear process modeling", Computers & Chemical Engineering, 30 (2006) 295-308.
10. J. Zhang, "Developing robust non-linear models through bootstrap aggregated neural networks", Neurocomputing, 25 (1999) 93-113.