RELIABLE MODELLING AND OPTIMISATION CONTROL OF REACTIVE POLYMER COMPOSITE MOULDING PROCESSES USING BOOTSTRAP AGGREGATED NEURAL NETWORK MODELS

Jie Zhang[1] and Nikos G. Pantelelis[2]
[1]School of Chemical Engineering and Advanced Materials, Newcastle University, NE1 7RU, Newcastle Upon Tyne, U.K.
[2]Department of Mechanical Engineering, National Technical University of Athens, Athens, Greece

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Abstract: This paper presents using bootstrap aggregated neural networks for the modelling and optimisation control of reactive polymer composite moulding processes. Bootstrap aggregated neural networks combine multiple neural networks developed from bootstrap re-sampling replications of the original training data in order to enhance model prediction and generalisation capability. Neural network models for modelling the degree of cure (through modelling the measured resistance) are developed from real industrial process operational data. Both static and dynamic models are developed and the developed neural network models are validated on unseen process operation data. The bootstrap aggregated neural network models give accurate and reliable predictions than single neural networks. Optimal heating profile is obtained by solving an optimisation problem using the dynamic neural network model. The model prediction confidence bound is incorporated in the optimisation objective function in order to enhance the reliability of the calculated optimal control profile. In addition to maximise the final degree of cure, model prediction confidence bound is minimised. Application results on a simulated polymer composite moulding process demonstrate that the proposed reliable optimisation control strategy is effective.

1 INTRODUCTION

Polymer composite materials have been increasingly used in many areas, for example, aerospace, automobile, and construction industries, due to their various advantages. For example, polymer composite is of much light weight and comparable strength compared with steel. Automobiles using polymer composite parts instead of steel parts will significantly save fuel consumption due to the much reduced weight. Polymer composite is corrosion resistant compared to steel making them ideal materials for many manufacturing industries. The curing of thermoset based polymer composite material is dominated by complex process dynamics and trial and error procedure is the only practical tool for process optimisation (Pantelelis, 2005).

Reactive polymer composite moulding processes are typical batch processes. The degree of cure is an important parameter in reactive polymer composite moulding processes. Only when the product is almost fully cured the mould can be opened. Thus, modelling the degree of cure is very important in the control and optimisation of reactive polymer composite moulding processes. Development of detailed mechanistic models for the degree of cure is generally time consuming and effort demanding. Data based empirical modelling can be a very useful alternative in this case. Neural networks have been shown to be capable of approximating any continuous nonlinear functions (Cybenko, 1989) and have been applied to nonlinear process modelling (Bhat and McAvoy, 1990); (Bulsari, 1995); (Su et al., 1992).

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 (Breiman, 1996); (Sridhar et al., 1996); (Zhang et al., 1997). The paper presents a study on using bootstrap aggregated

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neural networks for modelling the degree of cure and optimisation of polymer composite moulding processes.

The paper is organised as follows. Section 2 presents modelling of reactive polymer composite moulding process using bootstrap aggregated neural networks. Section 3 presents optimisation control of reactive polymer composite moulding process based the neural network model. Section 4 concludes the paper.

2 MODELLING OF REACTIVE POLYMER COMPOSITE MOULDING PROCESS USING NEURAL NETWORKS

2.1 Bootstrap aggregated Neural Networks

Neural networks have been shown to be capable of approximating any continuous nonlinear functions (Cybenko, 1989) and have been applied to nonlinear process modelling (Bhat and McAvoy, 1990); (Bulsari, 1995); (Su et al., 1992). In most of the reported applications, a single neural network is used to model the concerned nonlinear process. A limitation of single neural network models is that they can lack generalisation when applied to unseen data, i.e. the trained neural network gives good performance on the training data but gives unsatisfactory performance on unseen data which is not used in the training process. Several techniques have been reported in the literature for improving neural network generalisation capability, such as regularisation (Bishop, 1991), early stopping (Bishop, 1995), Bayesian learning (MacKay, 1992), training with both dynamic and static process data (Zhang, 2001), and combining multiple networks (Sridhar et al., 1996); (Wolpert, 1992); (Zhang et al., 1997). In training with regularisation, the magnitude of network weight is introduced as a penalty term in the training objective function in order to avoid unnecessarily large network weights which generally lead to poor generalization performance. In training with early stopping, neural network performance on the testing data is checked during the training process and the training process stops when the neural network prediction errors on the testing data start to increase. Among these techniques, combining multiple networks is a very promising approach to improving model predictions on unseen data. The emphasis of this approach is on generalisation accuracy on future predictions (i.e. predictions on unseen data). When building neural network models, it is quite possible that different networks perform well in different regions of the input space. By combining multiple neural networks, prediction accuracy on the entire input space could be improved. Bootstrap aggregated neural networks have been successfully used for the inferential estimation of polymer quality (Zhang et al., 1997), prediction of final product quality (Zhang et al., 1998), and estimation of reactive impurities and reactor fouling (Zhang et al., 1999) in a batch polymerisation process.

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.

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

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. Proper determination of the stacking weights is essential for good modelling performance. A popular choice of stacking weights is simple averaging, i.e. the stacked neural network output is an average of the individual network outputs. Since the individual neural networks are highly correlated, appropriate stacking weights could be obtained through principal component regression (PCR) (Zhang et al., 1997). Instead of using constant stacking weights, the stacking weights can also dynamically change with the model inputs (Ahmad and Zhang, 2005; 2006).

Another advantage of bootstrap aggregated neural network is that model prediction confidence bounds can be calculated from individual network predictions (Zhang, 1999). The standard error of the ith predicted value is estimated as

$$\sigma_e = \{\frac{1}{n-1}\sum_{b=1}^{n}[y(x_i;W^b) - y(x_i;\cdot)]^2\}^{1/2} \qquad (2)$$

where $y(x_i; .) = \sum_{b=1}^{n} y(x_i;W^b)/n$ and n is the number of neural networks in an aggregated neural

network. Assuming that the individual network prediction errors are normally distributed, the 95% prediction confidence bounds can be calculated as $y(x_i; .) \pm 1.96\sigma_e$. A narrower confidence bound, i.e. smaller σ_e, indicates that the associated model prediction is more reliable.

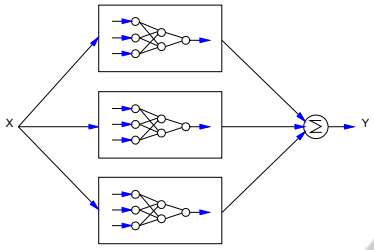

Figure 1: A bootstrap aggregated neural network.

2.2 Modelling the Degree of Cure in an Industrial Polymer Composite Moulding Process

Neural network models were developed using industrial data from an EU research project – iREMO (intelligent reactive polymer composite moulding). The process is for the manufacturing of car parts.

In the real reactive polymer composite moulding processes studied in this project, the curing process is monitored using OptiMould which measures resistance. The data set contains 6 runs at different moulding temperatures. Data from 4 runs were used to build neural network models and data from the other 2 runs were used as unseen validation data. The original data were sampled and stored at unequal sampling times due to the limitation in the sensor. For the purpose of neural network modelling, especially dynamic modelling, the data were re-sampled at equal sampling time. A sampling time of 30s were used.

Two types of neural network models were developed: a static model and a dynamic model. The static model is of the following form:

$$R(t) = f(t, T) \tag{3}$$

where $R(t)$ is the resistance at time t (min), T is the moulding temperature (^{o}C), and $f()$ is a nonlinear function represented by a neural network.

A bootstrap aggregated neural network containing 30 single hidden layer neural networks each with 12 hidden neurons was developed. The networks were trained with Levenberg-Marquardt algorithm (Marquardt, 1963) with regularisation and early stopping. Figure 2 shows the predicted resistance on the 2 unseen validation runs. In Figure 2, the actual measure resistances are shown as the solid lines whereas the neural network predictions are shown as dashed lines. The dotted lines are the 95% prediction confidence bounds. It can be seen that the neural network predictions are very accurate. Furthermore, the prediction confidence bounds are quite narrow, especially towards the end of the curing cycle where the model predictions are of more importance. This indicates that the bootstrap aggregated neural network gives accurate and reliable predictions. Thus it can be applied to the real industrial process with confidence.

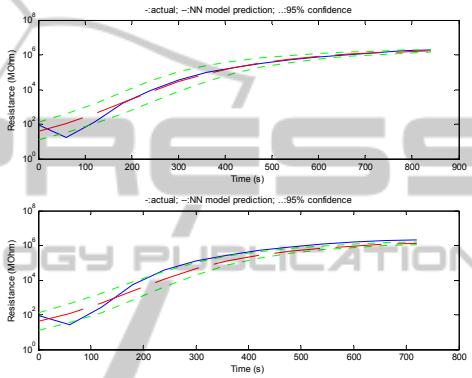

Figure 2: Static neural network model predicted resistance and the 95% prediction confidence bounds on the 2 unseen runs.

The dynamic model is of the following form:

$$y(t) = f[y(t\text{-}1), y(t\text{-}2), u(t\text{-}1)] \tag{4}$$

where y is the resistance, u is the applied temperature, 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 with 8 hidden neurons was developed. The networks were trained with Levenberg-Marquardt algorithm with regularisation and early stopping. Figure 3 shows the predicted resistance on the 2 unseen validation runs. In Figure 3, the actual measure resistances are shown as the solid lines, one-step-ahead predictions are shown as dashed lines, and multi-step-ahead predictions are shown as the dash-dotted 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. In contrast to the static model, predictions in the dynamic model can be updated using the online measured resistance. The static model, on the other hand, does not require measured

resistance as model input. When the measured resistance is affected by air bubble or carbon fibre, the dynamic model would not give good predictions and the static model can be used. Thus the two types of models can used in a complimentary way.

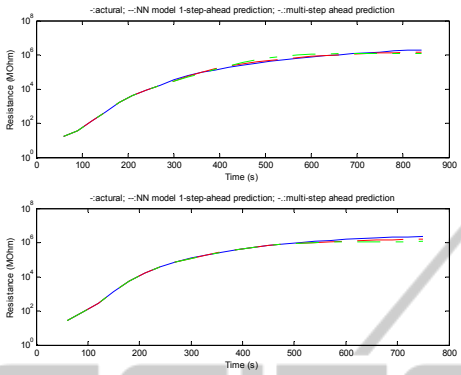

Figure 3: Dynamic neural network model predicted resistance on the 2 unseen runs.

3 RELIABLE OPTIMISING CONTROL

Using a neural network dynamic model, the optimal control profile (e.g. heating profile) is calculated off-line by solving the following optimisation problem.

$$\min_{u_1,\cdots u_N,t_f} J = w_1[\alpha_d - \alpha(t_f)] + w_2 t_f + w_3\sigma_e(t_f)$$

s.t. product quality and operation constraints

where α_d is the desired degree of cure, t_f is the batch time, σ_e is the standard error of neural network predictions, w_1, w_2 and w_3 are weighting factors, and $u_1,\ldots, u_N$ form the control profile. Earlier studies by Zhang (2004) and Mukherjee and Zhang (2008) show that penalising wide model prediction confidence bounds (i.e. large σ_e) leads to reliable optimal control policies.

The optimisation control strategy is tested on simulation using the mechanistic model given in (Pantelelis, 2005). The basic kinetic model is a combination of autocatalytic and nth order reaction terms with Arrhenius dependence of the rate constants:

$$\frac{da}{dt} = P_3 \exp\left(\frac{P_1}{R(T+273)}\right)(1-a)^{P_5} + P_4 \exp\left(\frac{P_2}{R(T+273)}\right)a^{P_6}(1-a)^{P_7} \quad (5)$$

where P_1 and P_2 are the activation energies, P_3 and P_4 are the rates constants, and P_5 to P_7 are the reaction orders. Two improved models incorporating glass transition temperature and a diffusion term are given in (Pantelelis, 2005). The improved model is used in this study and the model parameters can be found in (Pantelelis, 2005). From simulation, 7 batches were simulated and the sampling time is 4 minutes.

A dynamic neural network model was developed using 3 batches (batches 3, 5, 7) and the developed models are validated on 4 unseen validation batches (batches 1, 2, 4, 6). The developed model is a bootstrap aggregated neural network containing 30 neural networks. Each network is a single hidden layer feed forward neural network with 5 hidden neurons. The network was trained with Levenberg-Marquardt algorithm with regularisation and early stopping. Table 1 shows the mean squared errors (MSE) from one-step-ahead predictions and multi-step ahead predictions on the 4 unseen validation batches. It can be seen from Table 1 that the model predictions are very accurate.

Table 1: MSE of model predictions on validation data.

batch	1-step-ahead predictions	Long range predictions
1	0.0316×10^{-3}	0.2853×10^{-3}
2	0.0422×10^{-3}	0.2235×10^{-3}
4	0.1126×10^{-3}	0.1968×10^{-3}
6	0.0253×10^{-3}	0.2047×10^{-3}

In this study, the desired degree of cure is set to 1 and the constraints on the applied temperature are $20^oC \le T \le 160^oC$ and $0^oC \le \Delta T \le 70^oC$. The batch time is divided into several intervals each of 4 minutes and several possible batch times (in multiple of 4) were considered. Several batch ending times were considered and it is found that a batch time of 20 minutes is the shortest possible batch time. Two types of control profiles were considered: piecewise linear profile where the applied temperature linearly increases within each interval and piecewise constant profile where the applied temperature is kept constant within each interval. The optimisation problem is solved using sequential quadratic programming (SQP) implemented in the MATLAB Optimisation Toolbox. The SQP optimisation method mimics Newton's method for constrained optimisation in that at each major iteration an approximation is made of the Hessian matrix of the Lagrangian function using a quasi-Newton updating method. This is then used to generate a quadratic programming sub-problem which is solved and the solution is used to form a search direction for a line search procedure. The weighting parameter w_3 is selected as 0.1 in both cases.

Figure 4 shows the initial and optimised temperature profiles for the piecewise linear control profile and Figure 5 shows the corresponding degree of cure profiles. It can be seen from Figure 5 that the final degree of cure under the initial temperature profile is less than 0.9. Through optimisation based on the neural network model, the final degree of cure under the optimised temperature profile is 0.9866, which is very close to one.

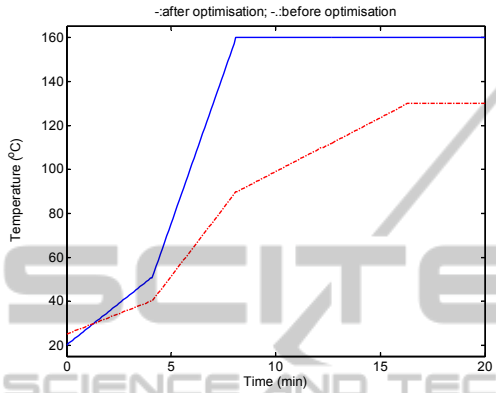

Figure 4: Temperature before (-.) and after (-) optimisation for the piecewise linear control profiles.

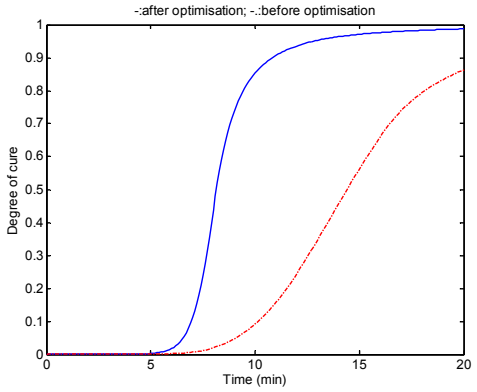

Figure 5: Degree of cure before (-.) and after (-) optimisation for the piecewise linear control profiles.

Figure 6 shows the initial and optimised temperature profiles for the piecewise constant control profile and Figure 7 shows the corresponding degree of cure profiles. It can be seen from Figure 7 that the final degree of cure under the initial temperature profile is less than 0.7. Through optimisation based on the neural network model, the final degree of cure under the optimised temperature profile is 0.9876, which is very close to one. The neural network predicted final degree of cure under this optimal curing temperature profile is 0.9722, which is very close to the actual value.

The results obtained demonstrate that the neural network models developed from polymer composite moulding process operation data can accurately represent the process and can be effectively used in finding the optimal temperature profile. The final degree of cure can be significantly improved through optimisation using the neural network models.

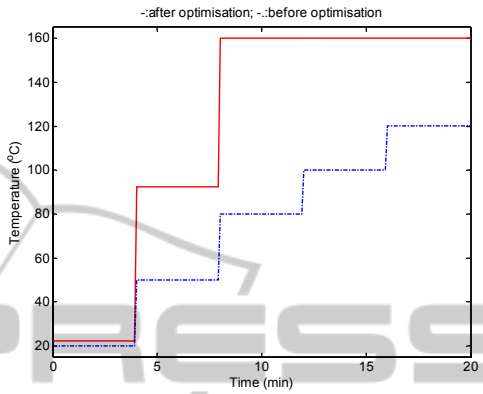

Figure 6: Temperature before (-.) and after (-) optimisation for the piecewise constant control profiles.

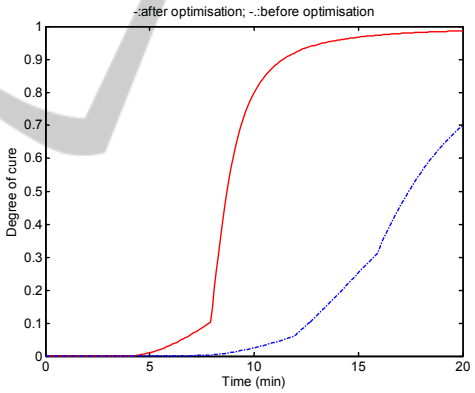

Figure 7: Degree of cure before (-.) and after (-) optimisation for the piecewise constant control profiles.

4 CONCLUSIONS

A reliable modelling and optimisation control strategy for reactive polymer composite moulding process based on bootstrap aggregated neural networks is presented in this paper. Application results on both simulated and real industrial data demonstrate that the developed neural network models can accurately predict the degree of cure (through predicting the measured resistance). In addition, model prediction confidence bounds are obtained from bootstrap aggregated neural networks. By incorporating the model prediction confidence

bounds into the optimisation objective function and penalising wide model prediction confidence bounds, reliable optimisation control policy is obtained. Application to a simulated reactive polymer composite moulding process demonstrates that the proposed reliable optimisation control technique is very effective.

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REFERENCES

Ahmad, Z. and J. Zhang, (2005). "Bayesian selective combination of multiple neural networks for improving long range predictions in nonlinear process modelling", *Neural Computing & Applications*, 14, 78-87.

Ahmad, Z. and J. Zhang, (2006). "Combination of multiple neural networks using data fusion techniques for enhanced nonlinear process modeling", *Computers & Chemical Engineering*, 30, 295-308.

Bhat, N. V. and T. J. McAvoy, (1990). "Use of neural nets for dynamical modelling and control of chemical process systems", *Computers & Chemical Engineering*, 14, 573-583.

Bishop, C., (1991). "Improving the generalisation properties of radial basis function neural networks", Neural *Computation*, 13, 579-588.

Bishop, C., (1995). *Neural Networks for Pattern* Recognition. Oxford University Press: Oxford.

Breiman, L., (1996). "Bagging predictor", *Machine Learning*, 24, 123-140.

Bulsari, A. B., (Ed), (1995). *Computer-Aided Chemical Engineering, Vol.6, Neural Networks for Chemical Engineers*, Elsevier: Amsterdam.

Cybenko, G., (1989). "Approximation by superposition of a sigmoidal function", *Math. Control Signal Systems*, 2, 303-314.

MacKay, D. J. C., (1992). "Bayesian interpolation", *Neural Computation*, 4, 415-447.

Marquardt, D., (1963). "An algorithm for least squares estimation of nonlinear parameters", *SIAM J. Appl. Math*., 11, 431-441.

Mukherjee, A. and J. Zhang, (2008). "A reliable multi-objective control strategy for batch processes based on bootstrap aggregated neural network models", *Journal of Process Control*, 18, 720-734.

Pantelelis, N. G., (2005). "Towards the dynamic optimisation for the cure control of thermoset-matrix composite materials", *Composites Science and Technology*, 65, 1254–1263.

Sridhar, D. V., R. C. Seagrave, and E. B. Bartlett, (1996). "Process modelling using stacked neural networks", *AIChE Journal*, 42, 2529-2539.

Su, H. T., T. J. McAvoy, and P. Werbos (1992). "Long-term prediction of chemical process using recurrent neural networks: a parallel training approach", *Ind. Eng. Chem. Res*., 31, 1338-1352.

Tian, Y., J. Zhang, and A. J. Morris, (2001). "Modeling and optimal control of a batch polymerization reactor using a hybrid stacked recurrent neural network model", *Ind. Eng. Chem. Res.*, 40, 4525-4535.

Wolpert, D. H., (1992). "Stacked generalization", *Neural Networks*, 5, 241-259.

Zhang, J., A. J. Morris, E. B. Martin, and C. Kiparissides, (1997). "Inferential estimation of polymer quality using stacked neural networks", *Computers & Chemical Engineering*, 21, s1025-s1030.

Zhang, J., A. J. Morris, E. B. Martin, and C. Kiparissides, (1998). "Prediction of polymer quality in batch polymerisation reactors using robust neural networks", *Chemical Engineering Journal*, 69, 135-143.

Zhang, J., A. J. Morris, E. B. Martin, and C. Kiparissides, (1999). "Estimation of impurity and fouling in batch polymerisation reactors through the application of neural networks", *Computers & Chemical Engineering*, 23(3), 301-314.

Zhang, J., (1999). "Developing robust non-linear models through bootstrap aggregated neural networks", *Neurocomputing*, 25, 93-113.

Zhang, J., (2001). "Developing robust neural network models by using both dynamic and static process operating data", *Ind. Eng. Chem. Res.*, 40, 234-241.