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NEURAL NETWORK CURE KINETICS MODELLING OF CARBON FIBRE SHEET MOULDING COMPOUND

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ABSTRACT

Sheet Moulding Compound (SMC) materials, renowned for their excellence in automotive and other industries due to their exceptional chemical and mechanical properties, have undergone advancements to refine their characteristics through innovative resin formulations and additives. However, obtaining precise formulation details remains challenging. This study addresses this gap by developing a cure kinetic model for a carbon fiber SMC material using Differential Scanning Calorimetry (DSC), without requiring detailed formulation information. Leveraging a neural network approach, the research aims to optimize manufacturing processes and enhance component properties. Experimental characterization, including isothermal and dynamic tests, facilitated the development of a robust regression model, exhibiting high agreement between predictions and observed data (R-squared value of 1 for train and test sets), as well as successful interpretation of unseen data and interpolation on the experimental conditions. These findings underscore the model's practical applicability in SMC manufacturing, opening avenues for further research in enhancing predictive accuracy and exploring alternative modeling techniques.

1 INTRODUCTION

Sheet Moulding Compound (SMC) materials have gained prominence in various industries, particularly automotive applications, due to their remarkable chemical and mechanical properties, alongside their efficient compression moulding manufacturing process [1]. Recent efforts by manufacturers and researchers have been directed towards enhancing SMC properties through the exploration of new resin formulations, integration of innovative reinforcements and additives, and the refinement of manufacturing processes to meet the evolving industry requirements [2], [3]. Central to optimizing SMC properties is a comprehensive understanding of cure kinetics, which governs the material's final properties and performance [4]. Traditionally, cure kinetics modeling has relied on empirical equations and experimental data obtained through techniques such as Differential Scanning Calorimetry (DSC) [5]. However, these conventional methods often necessitate detailed knowledge of the material's formulation, which may not always be readily available due to proprietary constraints. To address this challenge, advanced computational techniques, such as neural network modelling, have emerged as promising avenues for predicting cure kinetics without necessitating precise formulation details. Neural networks, renowned for their ability to discern intricate patterns from data, offer a flexible and data-driven approach to modelling cure kinetics, rendering them well-suited for applications in material science and engineering [6], [7].

The objective of this study is the development of a neural network-based cure kinetic model tailored to SMC materials. Leveraging neural network methodologies, the aim is to accurately predict the cure kinetics of SMC materials, thereby streamlining manufacturing processes and elevating component properties.

2 METHODOLOGY

A vinyl ester carbon based SMC, underwent extensive characterization despite its undisclosed formulation and the unavailability of resin separated from fibres provided by the manufacturer. Utilizing a modulated scanning calorimeter (MDSC) Q100 from TA Instruments, both isothermal and dynamic tests were conducted. Samples ranging from 5-12 mg of the compound were placed in aluminum hermetic pans and subjected to testing within a nitrogen environment. Isothermal tests were conducted at temperatures of 110 °C, 120 °C, and 130 °C, while dynamic tests were executed at constant heating rates ranging from 2.0 to 20.0 °C/min, covering a temperature range from 0 °C to 220-240 °C. Each experiment was conducted three times to mitigate variability. From these repetitions, two representative sets were selected and averaged for model training. The third repetition was set aside as a new dataset to assess the model's performance with unseen data.

Subsequently, the heat flow dH/dt was extracted from the MDSC datasets. The cure rate $d\alpha/dt$ was determined using Equation 1. The total heat of reaction H_t and the degree of cure α were crucial parameters, with the latter calculated by integrating the heat flow over the exothermic reaction time limits t_0, t, as defined by Equation 2.

$$\frac{d\alpha}{dt} = \frac{1}{H_t}\frac{dH(t)}{dt} \tag{1}$$

$$\alpha = \frac{H(t)}{H_t} = \frac{1}{H_t}\int_{t_0}^{t}\frac{dH(t)}{dt} \tag{2}$$

For dynamic tests, H_t was straightforwardly calculated by integrating the area under the heat flow reaction curve. In contrast, in isothermal tests, complete cure might not be achieved. Therefore, this value was determined as the combination of the heat observed during the isothermal scan H_{iso} and the residual heat from a subsequent dynamic scan H_{res} , $H_t = H_{iso} + H_{res}$.

2.1 Neural network

A supervised learning (SL) approach employing a backpropagation neural network (BPNN) was employed. This architecture ensures full connectivity between neighboring layers while avoiding connections within the same layer.

Data pre-processing has been demonstrated to enhance the accuracy and efficiency of training [8]. The input data X, including isothermal and dynamic averaged experiments, was normalized by shifting and scaling X to its mean value $\bar{X}$ and standard deviation σ as in Equation 3.

$$X_{norm} = \frac{X - \bar{X}}{\sigma} \tag{3}$$

Four input features were selected: time t, temperature T, heating rate dT/dt or isothermal temperature T_{iso} depending on the test type, and the degree of cure α. The cure rate $d\alpha/dt$ was chosen as the output feature and scaled to the range [0,1]. The dataset X was randomly partitioned into train (80%) and test (20%) sets, with an additional validation set for monitoring model performance during training.

A sequential model with five layers was built, incorporating three hidden layers with 12 neurons each, and it is schematized in Figure 1. Hyperbolic tangent (tanh) activation function $f_1 = \tanh(x)$ was chosen for the hidden layers, and a linear function $f_2 = x$ for the output layer [9]. The input data is fed into the input layer neurons, then it goes sequentially through the hidden layers until it reaches the output layer: this process is called forward propagation. The output of each neuron is combined to produce the total output of the neural network $\hat{y}$, as a function of the weights W^k, the output Z^k and the biases b^k of the layer k. If K is the index of the output layer, $\hat{y}$ can be calculated from Equation 4, where f_K is the activation function:

$$\hat{y} = Z^K = f_K(W^K \cdot Z^{K-1} + b^K) \tag{4}$$

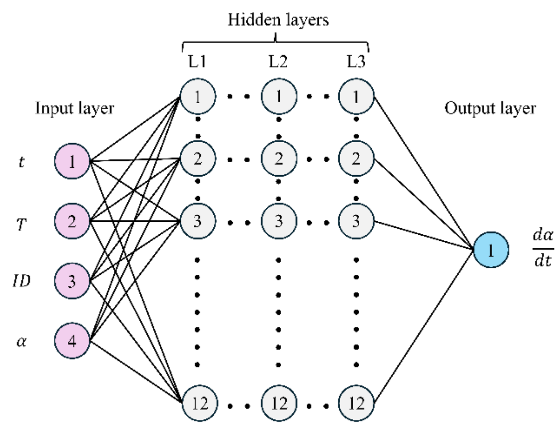


Figure 1. Neural network architecture.

After obtaining $\hat{y}$, i.e. after completing 1 epoch, the loss (error) between the predicted and the actual target value is calculated. Backpropagation calculates the gradients of the loss with respect to the weights and biases of the network, and then used to update the weights and biases using optimization algorithms such as stochastic gradient descent (SGD) or its variants. This iterative process of forward and back propagation continues until the network converges to a satisfactory solution or until a predefined number of epochs is reached. Adam optimizer was chosen due to its adaptative learning rate strategy, which ensures a rapid and stable convergence. The mean squared error (MSE) was selected as the loss function, which is commonly used for regression tasks due to its robustness in handling outliers. Mean absolute error (MAE) was employed as a metric to monitor the training process.

3 RESULTS AND DISCUSSION

The maximum number of epochs is set to 600, after previously training until 1500 and determining no significant improvement nor in the loss or validation loss values. The loss as a function of the number of epochs was captured and it is displayed in Figure 2, where the actual training ended after 555 epoch, from the monitoring validation loss value, which indicates the absence of overfitting. Values for MSE and MAE are shown in Table 1.

Table 1. Validation and training error for best epoch.

Epoch	Training MSE	Training MAE	Validation MSE	Validation MAE
555	$6.13 \cdot 10^{-6}$	$1.5 \cdot 10^{-3}$	$2.44 \cdot 10^{-6}$	$8.27 \cdot 10^{-4}$

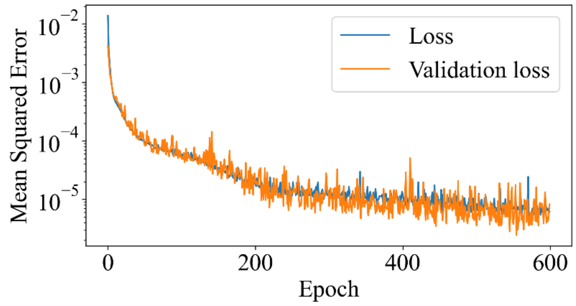
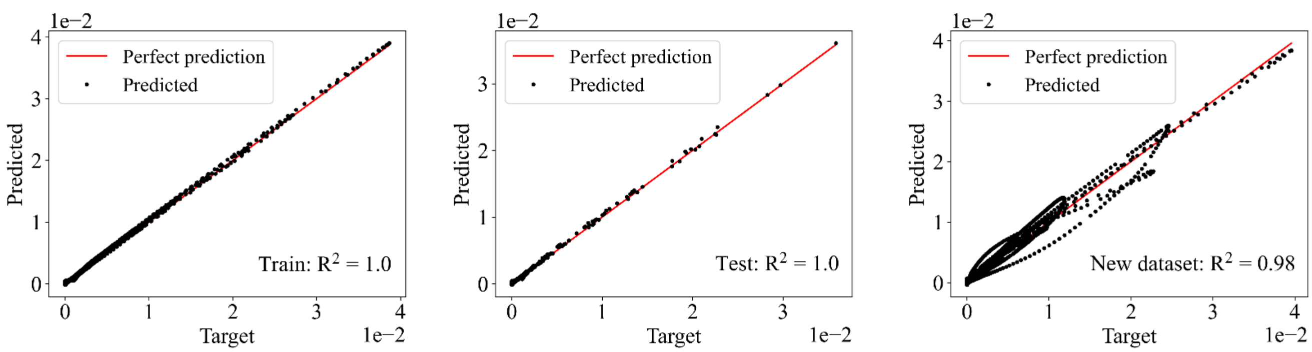


Figure 2. Neural network model convergence behaviour.

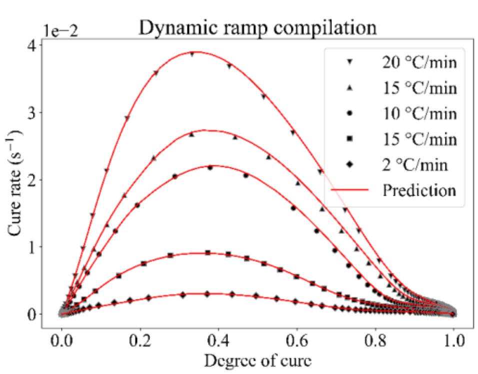
After training, a linear regression was used to evaluate the R-squared value (R^2) for both the test and train sets, along with new datasets (no averaged repetitions). These new datasets comprised experiments conducted under similar conditions (same time and temperatures) but were not part of the model's training data. The results are depicted in Figure 3. For the datasets used in the training process, including both the train (Figure 3. (a)) and test (Figure 3. (b)) sets, an R^2 value of 1 was obtained, indicating excellent agreement between the data and the model predictions. In the case of the new dataset (Figure 3. (c)), an R^2 value of 0.98 was achieved, demonstrating a slightly lower but still strong agreement compared to the test and train sets.



(a) (b) (c)

Figure 3. Linear regression for (a) train set, (b) test set, (c) new dataset.

Additionally, the cure rate was plotted against the degree of cure for the test set (Figure 4) and the new dataset (Figure 5), encompassing both isothermal and dynamic tests.



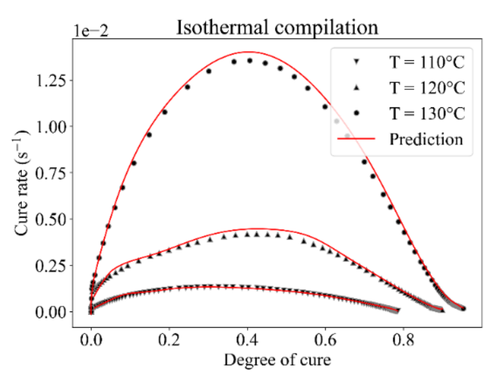


Figure 4. Predicted cure rate as a function of degree of cure for test set.

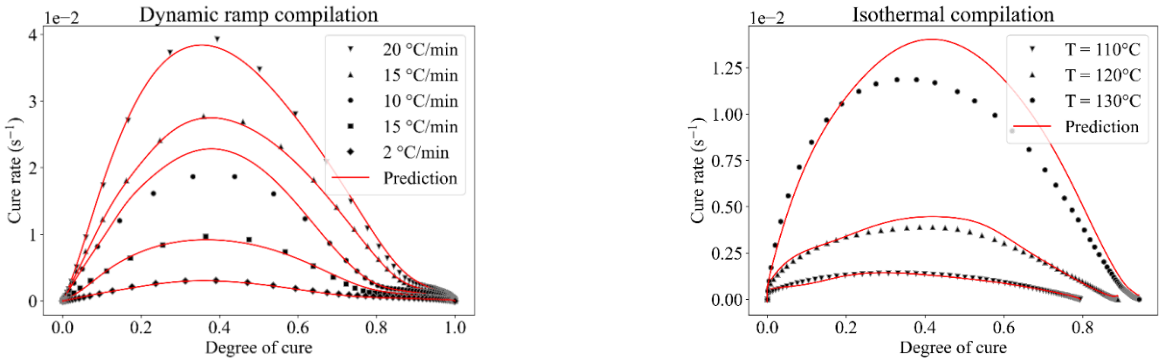
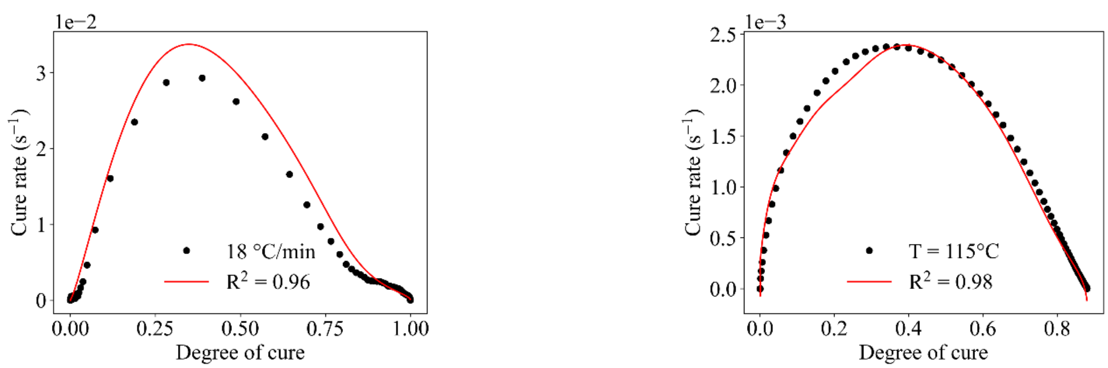


Figure 5. Predicted cure rate as a function of degree of cure for new dataset.

To assess the model's interpolation capacity, two new experiments were conducted using new experimental conditions: one isothermal test at T_{iso} of 115°C and one dynamic test with a heating rate dT/dt of 18°C/min. The results, shown in Figure 6, reveal R-squared values of 0.95 and 0.94 respectively, indicating good agreement between the observed data and the model's predictions.



(a) (b)

Figure 6. Cure rate as a function of degree of cure for, (a) 18 °C/min dynamic ramp experiment, (b) T = 116 °C isothermal experiment.

These findings suggest that the neural network model trained on the initial dataset generalizes well to new data, as evidenced by the high R-squared values obtained for the new datasets. Furthermore, the successful interpolation of the model to predict the cure rate under different experimental conditions underscores its robustness and utility. However, to deepen our understanding and potentially enhance the model's predictive performance, it may be beneficial to explore alternative modelling techniques. One intriguing avenue is to integrate the model to generate α and $d\alpha/dt$ with only time (t) and temperature (T) as inputs. This could be achieved through an iterative approach with an initial state or by employing a secondary auxiliary model. By doing so, it would be possible to assess how errors propagate through the model and identify the most effective method for predicting α and its derivative based solely on time and temperature inputs. This approach would not only provide valuable insights into the model's limitations and sources of uncertainty but also offer opportunities for refinement and optimization. Furthermore,

integrating such functionality into the model could enhance its practical utility, particularly in scenarios where direct measurement of α and $d\alpha/dt$ may be challenging or impractical, which is the norm in industrial work.
In summary, while the current linear regression model demonstrates promising performance, exploring innovative approaches such as integrating α and $d\alpha/dt$ prediction capabilities based solely on time and temperature inputs could lead to significant advancements in predictive accuracy and model applicability.

4 CONCLUSIONS

In conclusion, the study demonstrated the effectiveness of a linear regression model in predicting cure rate under varying experimental conditions. The high R-squared values obtained for both the training and new datasets indicate strong agreement between the model predictions and observed data, underscoring the model's robustness and generalization capability. Moreover, our findings suggest avenues for further investigation and model enhancement. Exploring alternative modeling techniques, such as nonlinear regression or machine learning algorithms, could offer opportunities for improving predictive accuracy and capturing complex relationships within the data.
Additionally, integrating the model to predict α and $d\alpha/dt$ based solely on time and temperature inputs presents an intriguing direction for future research. This approach not only facilitates error analysis and propagation but also enhances the model's practical utility in diverse experimental settings.

5 REFERENCES

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