RESIDUAL FOURIER NEURAL OPERATOR FOR THERMOCHEMICAL CURING MODELLING OF COMPOSITES

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ABSTRACT

During the curing process of composites, the temperature history heavily determines the evolutions of the field of degree of cure as well as the residual stress, which will further influence the mechanical properties of composite, thus it is important to simulate the real temperature history to optimize the curing process of composites. Since thermochemical analysis using Finite Element (FE) simulations requires heavy computational loads and data-driven approaches suffer from the complexity of high-dimensional mapping. This paper proposes a Residual Fourier Neural Operator (ResFNO) to establish the direct high-dimensional mapping from any given cure cycle to the corresponding temperature histories. By integrating domain knowledge into a time-resolution independent parameterized neural network, the mapping between cure cycles to temperature histories can be learned using limited number of labelled data. Besides, a novel Fourier residual mapping is designed based on mode decomposition to accelerate the training and boost the performance significantly. Several cases are carried out to evaluate the superior performance and generalizability of the proposed method comprehensively.

Keywords: Composites curing · Neural operator · Process simulation

1 Introduction

Composite materials, which consist of fibers (e.g. carbon fiber and glass fiber) embedded in polymer matrices (e.g. epoxy resin and unsaturated polyester resin), can provide higher structural performance (e.g. strength-to-weight ratio and corrosion resistance) than traditional metallic materials, and have been widely used in many fields including aerospace, automotive and renewable energy \cite{1} \cite{2}. To manufacture a composite structure, fibers impregnated with partially cured matrices are first cut and stacked to form a component of desired shape. This preformed component then have to be cured during which the matrices undergo the polymerization reaction initiated by heating following an appropriate cure cycle, to achieve the required mechanical properties \cite{3}. The cure cycle heavily determines the evolutions of the fields of temperature and degree of cure within the composite component which will further influence the residual stress field, thus it has to be seriously designed otherwise detects like incomplete cure, severe temperature overshoots, unacceptable levels of residual stresses and distortion may happen which will greatly degrade the performance of the final composite structure \cite{4} \cite{5}.

The model that maps cure cycles to the fields of temperature and degree of cure is essential for designing optimal cure cycles \cite{3}. Though the physics of the thermochemical curing process is well established and modeled by a set of coupled nonlinear partial differential equations (PDEs) describing heat conduction and resin cure kinetics, the closed-form solution is unavailable \cite{5}. Therefore, the fields of temperature and degree of cure nowadays are usually calculated

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by computational approximation like finite element method (FEM) \[6\]. But for parts with large size and complex structures, the computational efficiency of FEM is unable to meet the requirement for the iterative optimization of cure cycles in practical applications \[7\].

Recently, data driven models like neural network are researched to approximate the mapping by training with the data samples generated from expensive high-fidelity simulations with FEM \[8\][9]. These attempts are meaningful because an accurate data-driven surrogate model can greatly speed-up the optimization of curing process to minimize the risk in manufacturing \[10\]. Zobeiry et al. \[11\] established several data-driven models based on FE simulations to predict curing related parameters including steady-state thermal lag, transient thermal lag and exotherm. In their pioneering work, comprehensive domain knowledge was integrated into the components of neural network models to optimize feature transformation and activation function. To further reduce the data requirements, Ramezankhani et al. \[12\] proposed an interesting transfer learning framework to transfer the learned exotherm prediction model from one-hold cure cycle condition to two-hold cure cycle condition with only 500 simulated data for the target domain. Furthermore, they studied an active learning strategy to guide FEM simulation process so that the exotherm and thermal lag prediction models can be trained using only limited amount of data \[13\].

The researches mentioned above reveal that data-driven models are capable of achieving high accuracy result with small datasets in composite thermal analysis. However, these works focus on the prediction of some thermal parameters rather than the real temperature history of composites. Since the cure cycles and temperature histories are both functions of time and conventional machine learning methods can only build mapping from limit number of input features to few output features, it is difficult or impossible to train a high-dimensional mapping from the cure cycles to temperature or degree of cure histories directly. Therefore, cure cycles are usually simplified using few specific features including heat rate and top temperature, and the required temperature history is usually replaced by some representative parameters such as thermal lag and exotherm \[14][12\]. Keith et al. \[10\] represented the temperature histories and cure cycles as corresponding time series and designed a Long Short-Term Memory (LSTM) model to predict the temperature for each moment using time sequence evolution. However, the accuracy of this LSTM model relies heavily on a large amounts of simulation data (more than 100,000) generated by FEM software, which will restrict the application in real engineering scenarios.

Physics-informed Neural Networks (PINNs) emerge as an alternative approach to solve complex engineering problems \[15\]. By designing an integrated loss function based on PDE functions of the system, initial condition, and boundary condition, PINN can learn the underlying model by self-training without labelled data. Equations and conditions supervise the training instead of the traditional prediction error from labelled data \[16\]. Sina et al. \[17\] presented an elaborate PINN to simulate the fields of temperature and degree of cure of a composite-tool system. The coordinates of time and space are input features and the corresponding degree of cure and temperature can be predicted. Similarly, Zobeiry et al. \[11\] developed a PINN model to solve the temperature over the curing period and evaluated its effectiveness in several cases. Although these methods can solve heat transfer PDEs accurately subjected to the specific cure cycle, the model needs to be retrained completely for any new cure cycle, which cannot satisfy the requirements of cure cycles designing and optimization.

As reviewed above, it is still a great challenge to build a model to predict the entire temperature and the degree of cure histories for any given cure cycle because of the complexity of high-dimensional mapping. Recently, neural operators emerged as a new concept by generalizing standard feed-forward neural networks to learn mappings between infinite-dimensional spaces of functions without increasing the complexity of the network \[18\]. Based on the neural operator theory, this paper proposes a Residual Fourier Neural Operator (ResFNO) to establish the direct high-dimensional mapping from any given cure cycle to the corresponding temperature histories. A novel Fourier residual mapping is designed based on domain knowledge to accelerate the training and boost the performance. Several cases are carried out to evaluate the accuracy and generalizability of the proposed method comprehensively.

The remainder of the paper is organized as follows: The background of heat transfer problem of composite is introduced in section 2. The main framework of the proposed ResFNO is presented in detail in Section 3. Experimental results and analysis of 3 cases are provided in Section 4. The main conclusions are presented in the final section.

## 2 Background

The general form of exothermic heat transfer in composites curing process can be expressed as the following PDE:

\[
\rho C \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) + \dot{Q}
\]  

(1)
Where \( T \) is the temperature, \( \rho \) and \( C \) are density and specific heat capacity, and \( k \) indicates the thermal conductivity in specific direction. \( Q \) is the internal heat source, i.e. the rate of heat generation caused by the exothermic polymerization reaction in composite part, which is determined by instantaneous temperature and degree of cure. Besides, the initial conditions and boundary conditions are necessary for solving the PDE mentioned above. The typical boundary conditions include: Dirichlet boundary, Neumann boundary and Robin boundary.

- Initial condition:
  \[
  T_{t=0} = T_0; \alpha_{t=0} = \alpha_0
  \]  

- Dirichlet boundary:
  \[
  T_{x_b} = T_a(t)
  \]  

- Neumann boundary:
  \[
  k \frac{\partial T}{\partial x} \bigg|_{x_b} = q_{x_b}
  \]  

- Robin boundary:
  \[
  h (T_{x_b} - T_a(t)) = k \frac{\partial T}{\partial x} \bigg|_{x_b}
  \]

Where \( T_0 \) and \( \alpha_0 \) are the initial temperature and degree of cure and \( q \) is the flux density on the boundary. Equivalent to the air temperature in the autoclave and surfaces temperature in RTM (Resin transfer Molding), \( T_a(t) \) indicates the external temperature.

In this study, we start with an example of 1D composite-tool curing system with convective boundary conditions (Neumann boundary) in autoclave shown in Fig. 1(a). The heat transfer governing equation and boundary conditions can be formulated as:

\[
\rho C \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \dot{Q}
\]

\[
h_\ell (T_{x=0} - T_a(t)) = k \frac{\partial T}{\partial x} \bigg|_{x=0}
\]

\[
h_c (T_a(t) - T_{x=L_t+L_c}) = k \frac{\partial T}{\partial x} \bigg|_{x=L_t+L_c}
\]

Where \( h_\ell (h_c) \) is the heat transfer coefficient of composite (tool) and \( T_{x=0}, T_{x=L_t+L_c} \) is the temperature of composite-tool system at its lower (upper) surface. To guide the curing process, a cure cycle of air, i.e. \( T_a(t) \) depicted in Fig. 1(a), is designed to ensure the end-part quality. During the heat-up and cool-down stages, composite part temperature \( T_c(t) \) lags behind \( T_a(t) \) due to the thermal masses and thermal resistances of the part and tool [1]. However, as exothermic curing reaction starts within the part, \( T_c(t) \) gradually increases beyond \( T_a(t) \) and reaches the maximum temperature, as shown in Fig. 1(b). The temperature field directly determines the evolutions of the fields of degree of cure as well as the residual stress, which will further influence the mechanical properties of the cured composite, thus it is important to simulate the entire temperature history to optimize the curing process.

![Figure 1: Background of composites curing and problem definition](image-url)
As shown in Fig. 1(c), the purpose of this research is to build a surrogate model to predict the temperature histories $T_c(t)$ of all points on the composite-tool system for any given cure cycle function $T_a(t)$ accurately and effectively. Since the cure cycles and temperature histories are both functions of time, it is difficult or impossible to train a high-dimensional mapping from the cure cycles to temperature histories directly using conventional machine learning methods. Thus, the challenges of this research involve how to represent the input $T_c(t)$ and the output $T_a(t)$, how to integrate domain knowledge to accelerate the training, and how to learn an accurate prediction model using only limited simulation data.

3 ResFNO framework

As shown in Fig. 2, a Residual Fourier Neural Operator (ResFNO) framework is proposed to establish a direct mapping from the cure cycle $T_a(t)$ to the temperature history $T_c(t)$. In section 3.1, we introduce the typical Fourier Neural Operator method involving neural operator theory and Fourier layers, and explain how and why FNO can potentially predict the temperature history. In section 3.2, a novel Fourier residual mapping is presented to improve the typical FNO using domain knowledge.

3.1 Fourier Neural Operator

3.1.1 Neural Operators

When the cure period is discretized into finite number of time intervals, the cure cycle $T_a$ can be expressed by a vector sampled from the vector space of cure cycles over $\mathbb{R}^{n_t}$, where $n_t$ is the size of time intervals. Therefore, existing researches predict the temperature of subsequent time with LSTM by modeling the cure cycle as a discrete time series. From a more general perspective, both the cure cycle $T_a(t)$ and the temperature history $T_c(t)$ are functions sampled from two unknown temperature function spaces, thus the mapping from $T_a(t)$ to $T_c(t)$ can be treated as an operator between infinite dimensional function spaces. If the operator can be learned using a finite collection of input-output pairs $D = \{ (T_a(t)_1, T_c(t)_1), \ldots , (T_a(t)_n, T_c(t)_n) \}$, the temperature history $T_c(t)$ can be evaluated directly with a given cure cycle $T_a(t)^*$ rather than performing time-consuming simulation or series prediction. However, the mapping from $T_a(t)^*$ to $T_c(t)^*$ is a high-dimensional input-output task, which is a challenging machine learning problem because the number of parameters of the networks depends on the resolution of input data. High-resolution time domain data can greatly increase the complexity of the networks and the performance of the model will rely on huge amount of training data. Therefore, it is necessary to build a resolution-independent framework to learn high-dimensional mappings between functions.

Recently, neural operators emerged as a new concept by generalizing standard feedforward neural networks to learn mappings between infinite-dimensional spaces of functions [18]. Infinite-dimension means that the operators can process very high-dimensional mapping without increasing the complexity and the number of network parameters, which can bring a new solution for data-driven PDEs, including the heat transfer problems in composite curing. With the given collections of cure cycles, the learning process of neural operators could be regard as solving the empirical-risk minimization problem, which is equivalent as that of standard machining learning problem. The target function can be represented as:

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \| T_c(t)_i - G_{\theta}(T_a(t)_i) \|_u^2$$

(9)
Where $G_\theta$ is the neural operator parameterized by $\theta$. The concrete representation of $G_\theta$ is normally a series of linear operators and non-linear operators, including lifting layer, iterative kernel integration layer and projection layer.

As shown in Fig. 3, the input cure cycle is $T_a(t) \in \mathbb{R}^{d_t \times 1}$ where $d_t$ depends on the resolution of time intervals. This input structure seems consistent with traditional deep learning method. The great difference is that the dimension $d_t$ never participate the transformation operation in linear operators and non-linear operators. The lifting operator ($L$) and projection operator ($P$) are parameterized by two simple linear transformation $\theta_L \in \mathbb{R}^{1 \times n_w}$ and $\theta_P \in \mathbb{R}^{n_w \times 1}$, where $n_w$ is the width of the neural operator. The lifting operator aims to add more channels to enhance the representation capability of the neural network. In the next section, it will be further explained that the non-linear operators are also parameterized independent with $d_t$. Therefore, the complexity and size of parameters of the neural operator will not be influenced by the size of $d_t$ despite $d_t$ can be very large. This characteristic allows us to train the neural operator with low time-resolution dataset, and then predict on high time-resolution cure cycles. The neural operator from $T_a(t)$ to $T_c(t)$ can be treated as approximating the potential operator $G_\theta$ by linear combination of limited number of non-linear sub-operators:

$$g_\theta (T_a(t)) = \sum_{j=1}^{n_w} \theta_{Lj} \varphi_j(t) \theta_{Pj}$$

(10)

Where $\varphi_j(t)$ is the $j$-th iterative kernel integration, $\theta_{Lj}$ and $\theta_{Pj}$ are parameters of $j$-th channel in the lifting layer and projection layer.

3.1.2 Fourier Layer

Iterative kernel integration using Fourier layers are proven to be expressive enough to approximate any measurable operator mapping. The iterative updates process from Fourier layer $i$ to Fourier layer $i + 1$ can be simply represented as:

$$v_{i+1}(t) := \sigma (Wv_i(x) + R : \mathcal{F}v_i(w))$$

(11)

The detailed derivations of Fourier layer can be found in [2], which is not in the slope of this research. Here, we will introduce how and why Fourier layer is efficient to establish the mapping between the input cure cycle and the output temperature history. As shown in Fig. 4, a standard Fourier layer consists of five steps, FFT (Fast Fourier Transform), Low-pass filter, Linear transformation, IFFT (Inverse Fast Fourier Transform), and non-linear activation.

**Step1: FFT** Denote $v(t) \in \mathbb{R}^{d_t \times n_w}$ as the features after the lifting layer, $v(t)$ can be treated as $n_w$ time-domain functions $\{v^1(t), \ldots, v^{n_w}(t)\}$ because $d_t$ is the discrete size of the curing time. After FFT, time-domain functions for all channels are represented as $n_w$ frequency domain functions $\{\mathcal{F}^1(t), \ldots, \mathcal{F}^{n_w}(t)\}$. The frequency modes of the cure cycle functions can be extracted as new features of the neural network which can be more representative than purely time domain features. Note that, the number of parameters of the subsequent layers will also increase if all the frequency features are directly propagated to the next layer because the features after FFT is $\mathcal{F}(t) \in \mathbb{R}^{d_f \times n_w}$, where $d_f = 1 + d_t/2$.

**Step2: Low-pass filter** Normally, the cure cycles are characterized by heating stages, cooling stages and hold stages, and all these characteristics can be treated as low frequency features in the frequency domain. Therefore, it is reasonable to keep low frequency modes of $v(t)$ and abandon high frequency modes. Suppose $k$ lower modes are selected to propagate to next layer, the feature after low-pass filter is $\mathcal{F}_s(w) \in \mathbb{R}^{k \times n_w}$.
**Step 3: Linear transformation**
A linear transformation is parameterized for each channel as \( R^j \in \mathbb{R}^{k \times k} \) for \( j = 1, 2, \ldots, n_w \) so that the \( k \) input Fourier modes can be transferred to another appropriate \( k \) Fourier modes. The total linear transformation layer can be parameterized as a tensor \( R \in \mathbb{R}^{k \times k \times n_w} \), which is only dependent on the number of truncated Fourier modes \( k \) and the number of channels \( n_w \). The linear transformation in Fourier space can capture high-nonlinear features in the original space with resolution-invariant parameters.

**Step 4: IFFT**
Fourier features will be transformed to time domains by non-parametric IFFT operator. Then the feature becomes \( f^{-1}(\cdot)(t) \in \mathbb{R}^{k \times n_w} \) and the dimension returns to \( k \times n_w \).

**Step 5: Non-linear activation**
This step consists of a local linear transform \( W \) and an activation function, which play the same roles as in traditional full-connected neural networks. The activation function can be sigmoid, Relu, or tanh.

After the five-steps Fourier layer, the input feature \( v_i(w) \) become \( v_{i+1}(w) \). Normally, the Fourier layer will be repeated several times to strengthen the representative performance.

### 3.2 Fourier Residual Mapping

Typical FNO can be used to build high-dimensional mapping for different kinds of engineer problems as long as enough labeled data is available. However, it is expensive and time-consuming to collect the datasets of temperature histories both experimentally and computationally. In this section, a novel Fourier residual mapping is presented by combining the data-drive model and domain knowledge, thus the new framework can build the prediction model with high performance using only few data.

The first inspiration comes from the fact that the real temperature history is always highly correlated with the designed cure cycle. Although there are thermal lag and exotherm during heating, the basic shape and tendency over times are consistent. As analyzed in ResNet, it is easier to learn a residual function with reference to the input than learn an unreferenced function [19]. Denoting the underlying mapping from \( T_a(t) \) to the temperature history \( T_c(t) \) as \( G_\theta (T_a(t)) = G_\theta (T_a(t)) - T_a(t) \). From the perspective of function space, the original mapping \( G_\theta (T_a(t)) \) tends to be unrestricted and there are infinite number of potential solutions distributed over the whole function spaces. However, the mapping \( H_\theta (T_a(t)) \) is easier to learn because it is closer to zero mapping. As shown in Fig. 2, the residual mapping can be realized by FNO networks with a ‘shortcut connections’ from the input to the output.
Table 1: Material properties for AS4 fiber, 8552 epoxy and Invar tool

|                  | Volume fraction, \( v \) | Density, \( \rho \) (kg/m\(^3\)) | Specific heat capacity, \( C \) (J/kgK) | Thermal conductivity, \( k \) (W/mK) |
|------------------|---------------------------|--------------------------------------|------------------------------------------|--------------------------------------|
| AS4 fiber        | \( v_f = 0.574 \)         | \( \rho_f = 1790 \)                  | \( C_f = 914.0 \)                       | \( k_f = 3.960 \)                    |
| 8552 resin       | \( v_r = 0.426 \)         | \( \rho_r = 1300 \)                  | \( C_r = 1304.2 \)                      | \( k_r = 0.212 \)                    |
| Invar tool       | -                         | \( \rho_t = 8150 \)                  | \( C_t = 510.0 \)                       | \( k_t = 13.0 \)                     |

If we go deeper into the residual term \( r(t) = T_c(t) - T_a(t) \), one great challenge is that \( r(t) \) is non-differentiable because the cure cycle is a non-differentiable piecewise function. The residual term \( r(t) \) is represented by the black curve in Fig. 5(a) and the corresponding \( T_c(t) \) and \( T_a(t) \) are red curve and black curve in Fig. 5(b) respectively. It is obvious that there are 5 non-differentiable points on \( T_a(t) \) and \( r(t) \).

The output of FNO is differentiable because it is reconstructed by limited number of frequency modes. Therefore, there will be inevitable approximate error if we use a differentiable function to fit a non-differentiable function \( r(t) \). The predicted temperature history using direct residual FNO is shown as the blue curve in Fig. 5(b). There is a big prediction error (5.84 K) at the turning points of \( T_a(t) \) (around \( t = 160 \) min).

Inspired by the Fourier layer, a novel Fourier residual mapping is proposed to tackle the abovementioned challenge. As shown in Fig. 2, the original cure cycle \( T_a(t) \) can be transferred to a differential function \( T_F \) by reconstructing the signal using lower frequency modes. The number of modes can be the same with that in Low-pass filter in Fourier layer, namely \( k \). Then the Fourier residual can be represented as \( r_F(t) = T_c(t) - T_F \). The reconstructed cure cycle \( T_F \) and Fourier residual \( r_F(t) \) are shown as the green curve in Fig. 5(c) and Fig. 5(a) respectively. It is obvious that both functions become differentiable. The temperature history predicted using Fourier residual is shown as the blue curve in Fig. 5(c). It can be observed that the singular error in the non-differentiable point is greatly reduced.

The proposed framework ResFNO is simple but effective. It will be demonstrated in the following experiments that the integration of domain knowledge can reduce the testing error, accelerate the training process as well as reduce the requirements of training data.

### 4 Implementation and validation

#### Configuration of composites

To evaluate the performance of the proposed method, we consider a 1D exothermic heat transfer situation where an AS4/8552 composite part with a thickness of \( L_c = 20 \) mm, is placed on an Invar tool with a thickness of \( L_t = 30 \) mm. The material properties for AS4 fiber, 8552 epoxy and Invar tool are listed in Table 1. Given the densities and specific heat capacity of fiber and resin, the density \( \rho_c \) and specific heat capacity \( C_c \) of composite can be calculated via rules of the mixtures, i.e., Eq. (12) and Eq. (13). The thermal conductivity of the composite part in thickness direction can be obtained from Springer-Tsai model [20], as shown in Eq. (14), Eq. (15) and Eq. (16). Considering the complex flow field inside autoclaves, we assume convective boundary conditions with different heat transfer coefficients above composite part \( h_c = 120 \) W/m\(^2\)K and under the tool \( h_t = 70 \) W/m\(^2\)K.

\[
\rho_c = \rho_r v_r + \rho_f v_f \tag{12}
\]
\[
C_c = C_r v_r + C_f v_f \tag{13}
\]
Table 2: Detailed variable ranges of three temperature cycle cases

| Case   | ∆t (min) | ∆T (K) |
|--------|----------|--------|
| 1      |          |        |
|        | $t_1 \in (20, 80)$; $t_2 \in (t_1 + 20, 110)$;  | $T_0 = 293$ |
|        | $t_3 \in (t_2 + 20, 150)$; $t_4 \in (t_3 + 20, 190)$;  | $T_1 \in (50, 120)$ |
|        | $t_5 = 222$; $T_0 = 293$ | $T_2 \in (100, 240)$ |
| 2      | $t_1 \in (40, 90)$; $t_2 \in (t_1 + 30, t_1 + 90)$;  | $T_0 = 293$ |
|        | $t_3 \in (t_2 + 10, t_2 + 40)$; $T_1 \in (80, 140)$  | $T_1 \in (80, 140)$ |
|        | $t_4 \in (t_3 + 90, t_3 + 150)$;  | $T_2 \in (150, 170)$ |
|        | $t_5 = t_4 + T_2/2; t_6 = 500$  | $T_3 \in (80, 140)$ |
| 3      | $t_1 \in (30, 120)$; $t_2 \in (t_1 + 30, t_1 + 80)$;  | $T_0 = 293$ |
|        | $t_3 \in (t_2 + 10, t_2 + 30)$; $t_4 \in (t_3 + 10, t_3 + 20)$;  | $T_1 \in (140, 190)$ |
|        | $t_5 \in (t_4 + 30, t_4 + 60)$; $t_6 \in (t_5 + 90, t_5 + 150)$;  | $T_2 \in (30, 50)$ |
|        | $t_7 \in (t_6 + 20, t_6 + 60)$; $t_8 = 450$; $T_3 \in (80, 140)$ |

\[ k_c = k_r \left(1 - 2\Omega \right) + \frac{1}{\Gamma} \left(\pi - \frac{4}{r} \tan^{-1} \left(\frac{\sqrt{1 - \Gamma^2\Omega^2}}{1 + \Omega}\right)\right) \]  \hspace{1cm} (14)

\[ \Gamma = 2 \left(\frac{k_r}{k_f} - 1\right) \]  \hspace{1cm} (15)

\[ \Omega = \frac{\nu_f}{\pi} \]  \hspace{1cm} (16)

**Cure cycles of 3 cases** Three group of cure cycles are designed for the composite-tool system: extreme two-hold temperature cycle, realistic two-hold temperature cycle and smart cure temperature cycle [21]. The principles of designing cure cycles generally include heating rate, holding temperature, and holding time, which are relevant to heating methods and the resin type. Extreme two-hold temperature cycles generated by exaggerated process parameters don’t consider practical application, which is used to check the performance of the proposed method. As for realistic two-hold temperature cycles, we take the common heating rate range of autoclave, post-cure temperature and holding time into consideration. Smart cure cycles composed of cure-triggering, cooling and post-cure process are developed to reduce the thermal residual stress in some specific scenarios [21]. In this study, we set different variable ranges based on the temperature curve suggested by prepreg manufacturer. Moreover, we also replace the heating/cooling rate parameters with ‘heating time’ to simplify the generation of curves. Detailed variable ranges of three temperature cycles are listed in Table 2. All curves are generated by randomly selecting variables from predefined ranges. The results of schematic temperature cycles are depicted in Figure 1. The corresponding thermal histories of tool and composite are simulated in Comsol 5.4 software.

![Figure 6: Cure cycles for 3 cases](image-url)
Training settings  The proposed framework is implemented in Pytorch, which is a famous open-source machine learning library. The structure and parameters of the network are designed based on the experiences of Kovachki et al. [18], including 64 channels, 4 Fourier layers and 3 full-connected output layers. The sizes of frequency modes in Fourier layer and residual mapping are both 16. Other detailed hyperparameters can be found in the submitted source code. The loss function is defined as the relevant L2 norm between predicted the temperature history $T_{pre}(t)_i$ and the real temperature history $T_c(t)_i$:

$$
\text{loss}_{L2} = \frac{1}{n} \sum_{i=1}^{n} \frac{\|T_c(t)_i - T_{pre}(t)_i\|_2}{\|T_c(t)\|_2}
$$

All the experiments were carried out on an ordinary NVIDIA GeForce GTX 1660 SUPER GPU with 300 Epochs, a batch-size of 10, and a learning rate of 0.001. It is surprising that the training process only takes about 20 s and the prediction time can be negligible, thus the proposed method can be potentially used in online prediction during curing.

4.1 Experimental results of case 1

In this case, 200 extreme cure cycles are generated randomly, and the corresponding temperature histories of the tool and composite part are simulated in COMSOL. The thickness of the composite-tool system (50mm) is discretized into 51 elements and the total cure time (222min) is discretized into 223 elements. Firstly, we build the prediction model of the temperature history of the mid-point of the composite part, namely $x = 35$ mm. To check the influence of size of training data, 30, 50, 100 groups of samples $[T_c(t), T_c(t)_{x=35mm}]$ are randomly selected as training data to train FNO and ResFNO. The rest data are adopted as test data to study the generalization ability of the trained models. The convergences of train error and test error of FNO and ResFNO with different sizes of training data are shown in Fig. 6. It can be observed that ResFNO can converge quickly than FNO with different sizes of training data, and ResFNO can achieve much better performance with less training data. The relative L2 norm can be controlled below 0.01 with only 50 data. Considering the marginal gain of loss shows a progressive decrease with the increasing of training data. We will select 50 as the size of training data for the subsequent experiments.

![Figure 7: The convergent results for FNO and ResFNO with different sizes of training data](image)

Comparison between predicted temperature history  As the loss value cannot express the real fitting performance, 3 cure cycles in test datasets are randomly selected to test the prediction result explicitly. The designed cure cycle (T of Air), simulated temperature histories (T simulated) and predicted temperature histories (T FNO and T ResFNO) are depicted in Fig. 8. It can be observed that both methods can provide satisfactory goodness of fit. To further study the performance of the proposed method, a quantitative index is necessary to defined according to the application requirements. As the prediction error of temperature may influence the degree of cure and mechanical property of resin, the maximum absolute prediction error $\Delta T_{max}$ over the entire temperature history is selected to judge the prediction result. Compared with average prediction error shown in Fig. 7 $\Delta T_{max}$ is a strict criterion but more realistic for real application. As shown in Fig. 8 $\Delta T_{max}$ of FNO of 3 cure cycles are 10.28 K, 14.19 K, and 7.49 K respectively. By contrast, ResFNO can reduce the $\Delta T_{max}$ for all 3 cases to 4.75 K, 3.27 K and 1.41 K.

Predicted spatio-temporal temperature field  Abovementioned experiments result only focuses on $x = 35$ mm, namely the mid-point of the composite part. To predict the temperature history of the whole composite-tool system, we have to train 51 sub-models from $x = 0$ mm to $x = 51$ mm. The training effort is completely acceptable because the training process of one sub-model only takes about 20 s in a PC with GeForce GTX 1660 S GPU. The temperature histories of the whole composite-tool system predicted by FEM and ResFNO are shown in Fig. 9(a) and Fig. 9(c).
The range of prediction error for all 150 test cure cycles are reduced to results with density of \( \Delta \) points in Fig. 12(a) are less than 56. Figure 9: Comparison between the predicted temperatures and the simulation results for case 1

Statistical analysis of prediction results As Fig. 9 can only show the prediction results for one cure cycle, comprehensive statistical results are provided in Fig. 11 and Fig. 12 to further analyze the performance of the proposed ResFNO. The color map of prediction errors of all 150 test cure cycles at \( x = 35 \text{ mm} \) is shown in Fig. 11(a). And the colormap of prediction errors of \( x = 0 \text{ mm} \) to \( x = 51 \text{ mm} \) for one cure cycle is shown in Fig. 11(d). The probability density of \( \Delta T \) and \( \Delta T_{\text{max}} \) of the two colormaps are shown in Fig. 11(b, c, e, f). It can be observed in Fig. 11 that the range of prediction error of FNO is \(-22.5 \text{ K} \) to \(+18 \text{ K} \). Only 44.39% cure cycles can obtain satisfactory prediction results with \( \Delta T_{\text{max}} < 6 \text{K} \). By contrast, the prediction errors of ResFNO are much less than FNO as shown in Fig. 12 The range of prediction error for all 150 test cure cycles are reduced to \(-8 \text{K} \) to \(+6.4 \text{K} \). Besides, the prediction errors of 96.19% points in Fig. 12(a) are less than \( \pm 2 \text{K} \), and 82.06% cure cycles can be predicted with \( \Delta T_{\text{max}} < 6 \text{K} \). More indicators about prediction error can be found in Fig. 11 and Fig. 12. It is clear that ResFNO can provide more accurate and stable prediction results compared with FNO.
4.2 Experimental results of case 2

In this case, we will analyze the performance of ResFNO with more realistic cure cycles. These cure cycles are generated considering many physical constraints such as heating rate range of autoclave, post-cure temperature, holding time et. al. Most of experimental configure are the same with case 1 including 50 training samples, 150 test samples and 51 discretized elements in the thickness direction of the composite-tool system. One difference is the variant curing time from around 270 min to 420 min. Additional indoor temperatures (293 K) are added to the time series of cure cycles to ensure the identical size of \( T_n(t) \), namely 500 min discretized into 501 elements. The temperature histories of the composite-tool system predicted by FEM and ResFNO are shown in Fig. 13(a) and Fig. 13(c) respectively. And the predicted temperature histories for \( x = 35 \text{ mm} \) and \( x = 21 \text{ mm} \) are shown in Fig. 13(b) and Fig. 13(d) respectively. The predicted results of ResFNO are awesome and the maximum prediction errors are only 2.93\( K \) and 2.72\( K \). The predicted results of degree of cure are provided in Fig. 14. The maximum prediction errors for \( x = 21 \text{ mm} \) and \( x = 51 \text{ mm} \) are within the acceptable range 0.02.

The statistical analysis of prediction error of ResFNO are shown in Fig. 15. The prediction errors of more than 98% points in all 150 test cycles at \( x = 35 \text{ mm} \) are less than \( \pm 2K \). And almost all points from \( x = 0 \text{ mm} \) to \( x = 51 \text{ mm} \) for the selected cure cycle show errors less than \( \pm 2K \). More than 96%\( \Delta T_{\text{max}} \) are less than 6\( K \) besides few special cure cycles.
Figure 12: Statistical analysis of prediction errors of ResFNO for case 1

Figure 13: Comparison between the predicted temperatures and the simulation results for case 2

4.3 Experimental results of case 3: transfer learning

Case 1 and Case 2 have demonstrated that ResFNO can provide satisfactory prediction results for classical two-hold cure cycles. In this case, we will explore the generalizability and transferability of the trained ResFNO in special smart cure cycles. Firstly, we train a ResFNO model using 50 samples in case 1, then predict the temperature of a smart cure cycle to evaluate if the trained model can be generalized to more broader distribution. As shown in Fig. [16](a), the predicted result is extremely terrible and $\Delta T_{\text{max}}$ reaches 33.06 K. The result mean that ResFNO model trained on 50 two-hold samples can only be used to prediction cure cycles from similar distribution.

Traditional machine learning method can maintain its effectiveness only when all training data and test data follow the same distribution. When the distribution of target domain is different from the source domain, transfer learning methods can adapt the distribution discrepancy with few labelled target data [22]. Therefore, 10 smart cure cycles and the corresponding temperature histories are selected as target data to finetune the ResFNO network trained in case 1. Considering the special structure of ResFNO, we designed three finetuning strategies, including finetuning dense layers (Lifting and Projection layers), finetuning Fourier Layers, and finetuning all parameters.

As shown in Fig. [16](c), $\Delta T_{\text{max}}$ of the predicted temperature history after finetuning dense layers is reduced to only 4.24 K. The statistical analysis results of 40 complex smart cure cycles are shown in Table. 3. It can be observed that transfer learning can improve the prediction results to some extent and finetuning dense layers seems to be the best.
strategy. The average $\Delta T_{\text{max}}$ of 40 cycles after finetuning dense layers is around 8.64 K. To be honest, the prediction results are not as satisfactory as case 1 and case 2 because of the extreme complex cure cycles and few available data. But these experiments show the potential of transfer learning for ResFNO, which will be our next concerned topic.

### Table 3: Statistical analysis of $\Delta T_{\text{max}}$ on different transfer learning strategies

| Strategy                  | Mean and Standard deviation of $\Delta T_{\text{max}}$(K) |
|---------------------------|----------------------------------------------------------|
| Generalization            | 35.96(6.25)                                              |
| Target data only          | 13.39(4.79)                                              |
| Finetune Fourier layers   | 9.54(3.31)                                               |
| Finetune dense layers     | 8.64(2.61)                                               |
| Finetune all parameters   | 9.68(3.37)                                               |
5 Conclusion

During the curing process of composites, the temperature history directly determines the evolutions of the field of degree of cure as well as the residual stress, which will further influence the mechanical properties of composite, thus it is important to simulate the real temperature history to optimize the curing process of composites. A Residual Fourier Neural Operator framework is proposed to establish a direct mapping from the cure cycle $T_a(t)$ to the temperature history $T_c(t)$. Several case studies have evaluated the significant performance of the proposed method. Some conclusions can be drawn as follows:

- It is effective to model the mapping between the cure cycle to the temperature history using neural operators because the two temperature functions can be decomposed into limited number of modes in frequency domain.
- By incorporating the domain knowledge into neural operators, the proposed ResFNO can provide more accurate prediction results, accelerate the training process as well as reduce the requirements of training data.
- According to the experimental results of case 3, the proposed ResFNO has shown the potential to transfer the learned knowledge to more complex scenario.

It will be of further interest to apply ResFNO to more complex settings including changing heat transfer coefficient and spatial-temporal field prediction, with the aim of developing more effective and general thermal modelling methodologies.

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