Prediction of the Temperature of Large Framed Mold and Curing Deformation of Composite Components in the Autoclave Process

Zhipeng Wu, 1 Anan Zhao, 1 Ming Yue, 2 Jungang Guo, 2 Qing Wang 3, 1 and Yinglin Ke 1

1 School of Mechanical Engineering, Zhejiang University, Hangzhou 310027, China
2 AVIC Xi’an Aircraft Industry (Group) Company Ltd., Xi’an 710089, China

Correspondence should be addressed to Qing Wang; wqing@zju.edu.cn

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1. Introduction

Advanced composite materials have been widely used in aerospace field due to their excellent properties, such as high specific stiffness, high specific strength, and corrosion resistance [1, 2]. One of the popular processing methods adopted in composite manufacturing industry is the technology of autoclave molding since this technology produces the highest quality of the part. However, autoclave processing inevitably results in residue stress and process induced deformation of composite parts [3, 4], and further influences the physical and structural properties of the composites [5].

Considerable efforts have been made to investigate process-induced deformation for the precise manufacturing of composite parts, and finite element modeling (FEM) has been found to be a helpful tool in the composite manufacturing industry [6, 7]. For now, FEM on the forming process of composite materials has been vigorously researched, and some sophisticated constitutive models have been proposed. A typical FEM numerical simulation consists of the heat transfer-curing model and the stress-deformation model [8].

The heat transfer-curing model predicts the complex heat flow field and the temperature distribution of composite parts. The heat flow field in an autoclave is the main reason for the uneven temperature distribution of composite tooling, and considerable research on this topic has been reported. Dolkun et al. [9] established a computational fluid dynamics (CFD) based autoclave simulation model to investigate the influence of mold placement variation in an autoclave on the heating performance of a large framed tool and find the optimal mold placement parameters for improving the temperature uniformity and heating rate. Wang et al. [9, 10] developed an optimization process combining numerical simulations with a greedy genetic algorithm to realize the optimal layout and geometry of the local-isolation structure in molds, and finally, achieve a more uniform heating condition and more synchronous curing process. Zhang et al. [11] developed a reliable CFD simulation model considering the fluid-thermal-solid interaction inside the autoclave and used the single-variable method to study the effects of the material thermal properties on the temperature performance of large framed molds. The aforementioned studies have drawn the conclusion that the temperature on
the mold surface is distributed unevenly and shows a large gradient distribution in the process of autoclave forming. However, the effect of the uneven temperature distribution of composite tooling on the curing-induced deformation still needs to be further investigated.

On the other hand, the stress-deformation model adopts the temperature distribution from the heat transfer-curing model to simulate the temperature history of the fiber-reinforced polymer based on the heat transfer equation [12, 13]. This model also takes chemical shrinkage and thermal expansion into consideration [14]. In the aspect of constitutive material modeling, the linear elastic model [15], the path-dependent model [16], and the viscoelastic model [17] are representative models. Based on the stress-deformation model, a great number of investigations have been carried out to analyze the residue stress and deformation of composite parts. However, research on the forming process of large-scale composite components with complex tooling is still lacking.

Due to the complex structure of the frame mold, the temperature of the mold surface is not uniform, and the temperature gradient is generated. It causes the composite material component to be cured asynchronously during the molding process, which affects the molding performance of the component. To this end, the present paper takes the composite frame mold in the autoclave forming process into consideration. Firstly, based on the commercial software CFX, the calculation model of the heat flow field and temperature field is established to obtain the temperature field data of the autoclave process. Then, the temperature field is used as the temperature load of the composite component. The temperature field and curing deformation of the component in the actual forming process are calculated. The calculation results are compared with those obtained under the ideal temperature condition. The influence of the uneven temperature field of the mold on the curing deformation of the component is analyzed. The research work can provide a scientific design basis for composite mold designers.

2. Mold Temperature Field Analysis

2.1. Frame Mold Structure. The research object of this paper is the frame-type mold, which is widely used in the aviation composite material manufacturing industry. It is composed of a molded panel, support grid, vents, and temperature holes. The mold size simulated in this paper is 8000 mm × 2000 mm × 462 mm, the surface thickness is 12 mm, the support frame number is 6, the vent size is 180 mm × 260 mm, and the uniform temperature hole size is Φ80 mm. The three-dimensional model of the mold is shown in Figure 1, the length direction is the X direction, the width direction is the Y direction, and the height direction is the Z direction.

2.2. CFX Modeling and Numerical Calculation. A 10m autoclave of an aircraft manufacturer is used as a prototype, and the working cavity of the autoclave model is simplified into an approximate cylinder. Its radius is 2.5 m and the bottom edge is 3.1 m. The simplified autoclave section is shown in Figure 2. Figure 3 shows a simplified model of the composite material forming mold and the autoclave. The gas enters from the left end of the cylinder and exits from the right end.

The material of the mold is INVAR alloy, and the thermal conductivity is shown in Table 1.

The temperature process curve of the autoclave is shown in Figure 4. The constant flow velocity at the inlet boundary of the autoclave \( v = 4 \) m/s, and the pressure is 0.6 MPa.

The temperature field numerical simulation model constructed in this paper is similar to the model constructed in the literature [18, 19]. However, the model in this article predicts the distribution of the three-dimensional temperature field of the mold in the autoclave.

2.3. Governing Equation

2.3.1. Fluid Region. The whole autoclave is divided into two regions: fluid and solid. The fluid flow and heat transfer phenomena in the fluid region are controlled by the conservation laws of mass, momentum, and energy. The differential form of the three conservation equations in Cartesian coordinates is as follows:

(1) Mass conservation equation

\[
\frac{\partial \rho}{\partial t} + \text{div} (\rho \mathbf{v}) = 0, \tag{1}
\]

where \( \rho \) is the density of fluid, \( \mathbf{v} = [u, v, w]^T \) is the velocity vector of fluid, \( u, v, \) and \( w \) are, respectively, the components of velocity in \( x, y, \) and \( z \) directions.

(2) Momentum conservation equation

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \text{div} (\rho \mathbf{v} \otimes \mathbf{v}) = \text{div} (\mu \text{grad} \mathbf{v}) - \text{grad} (p) + \mathbf{S}, \tag{2}
\]

where \( \mu \) is the dynamic viscosity of the fluid; \( p \) is fluid pressure; and \( \mathbf{S} \) is the source term of the generalized momentum equation.

(3) Energy conservation equation

\[
\frac{\partial (\rho h)}{\partial t} + \text{div} (\rho h \mathbf{v}) = \text{div} (\lambda \text{grad} T) - p \text{div} \mathbf{v} + \Phi + S_h, \tag{3}
\]

where \( h = h(p, T) \) is the function of fluid pressure and fluid temperature; \( \lambda \) is the thermal conductivity;
Φ is the energy of viscosity dissipation; and \( S_h \) is the internal heat source.

There are 6 unknowns in equations (1)–(3): \( u, v, w, \rho, T, \) and \( p \), to set up a closed-form equation system add a relationship between \( p \) and \( q \):

\[
\rho = f(\rho, T).
\]

2.3.2. Solid Region. The control equation in the solid region is relatively simple, it obeys the law of conservation of energy:

\[
\frac{\partial (\rho c T)}{\partial t} = \text{div} (\lambda \text{div} T) + S_T,
\]

where \( \rho_s \) is solid density, \( c_s \) is solid specific heat capacity, \( T \) is solid temperature, and \( S_T \) is the internal heat source.

2.4. Temperature Field Simulation Results. The above process parameters were used to simulate the temperature field of the frame mold shown in Figure 1 based on Ansys CFX. The temperature field analysis results of frame mold at different process temperatures as shown in Figures 5–7. The numerical value is Kelvin temperature.

Simulation results show uneven temperature distribution. At the end of the process temperature rise stage, due to the fact that the temperature rise has just ended, it has a large surface temperature difference. The windward side of the mold (left side) is 28°C higher than the leeward side. The lowest point of the mold surface temperature exists under the right side of the frame profile, the temperature is only 78.90°C, as shown in Figure 5. However, at the end of the process heat preservation stage, the temperature uniformity has been greatly improved. The difference in the surface temperature of the frame mold is only about 3°C, as shown in Figure 6. In the cooling stage (Figure 7), the surface temperature distribution of the frame mold is opposite to the heating process. The low-temperature zone of the frame mold appears on the windward side of the mold (left side), and the high-temperature zone appears on the leeward side of the frame mold. The temperature difference is also relatively large, which can reach 90°C.

From the above analysis, it can be seen that for a large frame-type mold, the surface has a temperature gradient during the molding process. Since the composite component is in direct contact with the mold surface, this article focuses on the analysis of the temperature field of the mold surface. The two endpoints and the middle point along the diagonal of the profile were chosen for analysis. The temperature change curve is shown in Figure 8. It can be seen that there is a delay in the temperature change during the molding process, the temperature at endpoints rises fastest, and the
3. Analysis of Temperature Field and Curing Deformation

3.1. Temperature Field Calculation Model. During the curing process, the heat transfer reaction and the chemical reaction proceed simultaneously. The temperature of the composite material is determined by the internal temperature of the autoclave, the heat transfer performance of the mold, and the heat released by the curing reaction, which is equivalent to a nonlinear temperature transfer problem with an internal heat source. The expression of the heat transfer model used in this paper is as follows [8, 20]:

\[
\rho C \frac{dT}{dt} = \frac{\partial}{\partial x} \left( k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) + q. \tag{6}
\]

where \( \rho \) is the density of the composite material, \( C \) is the specific heat capacity, \( T \) is the current temperature of the curing reaction, \( k_i \) \((i = x, y, z)\) represents the thermal conductivity of the anisotropic material in three directions, and \( q \) is the internal heat source and can be obtained

\[
q = \rho_c V_r H_r \frac{\partial \alpha}{\partial t}, \tag{7}
\]

where \( \rho_c \) is the density of resin, \( V_r \) is the volume fraction, \( H_r \) is the total heat from the resin curing reaction of unit mass, and \( \frac{\partial \alpha}{\partial t} \) is the curing reaction rate of prepreg, which is expressed by the following curing kinetics equation:

\[
\frac{\partial \alpha}{\partial t} = A_1 \exp \left( -\frac{E_1}{RT} \right) \alpha^m (1 - \alpha)^n_1 + A_2 \exp \left( -\frac{E_2}{RT} \right) (1 - \alpha)^m_2, \tag{8}
\]

where \( A \) is the frequency factor, \( E \) is the reaction activation energy, \( R = 8.3145 \), which is the universal gas constant, \( T \) is the absolute temperature, and \( m \) and \( n \) are the model reaction order.

In the composite material component molding, this paper uses single-platform curing. In the heating and cooling stage, we use the model parameters at a rate of 3°C/min. In the heat preservation stage, we use the model parameters at a rate of 1°C/min.

3.2. Calculation Model of Curing Deformation. In the molding process of composite materials, their thermodynamic properties are constantly changing. When calculating the cure-induced deformation, UMAT is used to define the material’s elastic modulus, Poisson’s ratio, and other mechanical parameters, and the Jacobian matrix of the material is defined in the subroutine to calculate the stress and strain.

In this paper, a self-consistent method [20] is used to express the time-varying characteristics of a material parameter. The elastic constants of unidirectional fiber composites are as follows, where \( m \) and \( f \) represent resin and fiber materials and subscripts 1, 2, and 3 represent the direction of three spindles of unidirectional composites.

Longitudinal elastic modulus

\[
E_1 = 5000 \text{ GPa}
\]

Transversal elastic modulus

\[
E_2 = 2000 \text{ GPa}
\]

Poisson’s ratio

\[
\nu = 0.3
\]

Shear modulus

\[
G_1 = 1500 \text{ GPa}
\]
\[ E_1 = E_{f1}V_f + E_m(1 - V_f) \]
\[ + \frac{4(v_m - v_{f12})K_fK_mG_m(1 - V_f)V_f}{(K_f + G_m)K_m + (K_f - K_m)G_mV_f}. \]

(9)

Transverse elastic modulus
\[ E_2 = E_3, \]
\[ = \frac{1}{4K_r + 1/4G_{23} + v_{12}^2/E_1}, \]
with
\[ K_r = \frac{K_m(K_f + G_m) + G_mV_f(K_f - K_m)}{(K_f + G_m) - V_f(K_f - K_m)}. \]

(10)

Longitudinal Poisson’s ratio
\[ \nu_{12} = \frac{v_{12}V_f + v_m(1 - V_f)}{2E_fK_r - E_fE_2 - 4v_{12}E_2K_r}. \]

(12)

In-plane shear modulus
\[ G_{12} = G_{13} \]
\[ = \frac{G_m(G_{f12} + G_m) + (G_{f12} - G_m)V_f}{G_m(G_{f12} + G_m) - (G_{f12} - G_m)V_f}. \]

(14)

Transverse shear modulus
\[ G_{23} = G_m \cdot \frac{K_m(G_m + G_{f23}) + 2G_mG_{23} + K_m(G_{f23} - G_m)V_f}{K_m(G_m + G_{f23}) + 2G_mG_{f23} - (K_m + 2G_m)(G_{f23} - G_m)V_f}. \]

(15)

The bulk modulus \( K \) can be expressed as follows:
\[ K = \frac{E}{2(1 - v - 2v^2)}. \]

(16)

3.3. Curing Deformation Analysis Based on Finite Element Method. In this paper, ABAQUS software is used to solve the cure-induced deformation of the component, and the subroutines for calculating the temperature field and the degree of the cure field are written in Fortran language. Calculation of curing deformation is completed by UMAT and UEXPAN. The calculation process is as follows:

First define the field variables of the initial curing degree and curing rate through USDFLD, then establish the time-varying model of specific heat and thermal conductivity in UMATHHT [8]. The temperature boundary conditions and environmental convection of the finite element model are added to DISP and FILM. In this paper, the temperature boundary condition is obtained by calculating the temperature field of the mold, which is different from the traditional method.

The obtained temperature field results are substituted into the Jacobian matrix, combined with the thermal expansion defined by UEXPAN, and the stress and strain are finally calculated.

3.4. Cure-Induced Deformation Simulation of Composite Components. This paper analyzes the panel formed by the above frame mold, and its structure is shown in Figure 9. The overall length of the composite panel is 8 m, the width is 2 m, and the thickness is 5 mm. The prepreg material is a unidirectional strip, and the paving sequence is [0/45/90/-45]_5s.

This article uses T300/epoxy resin material [24], the resin volume fraction is 0.35, the total reaction heat of the resin in the curing reaction process is 120.25 KJ/kg, the curing kinetic model parameters are shown in Table 2, where the activation energy of the two reactions are respectively 58.5 KJ/mol and 81.157 KJ/mol. The law of mixing is used to express the time-varying characteristic of the thermodynamic parameters. The thermal conductivity and expansion coefficient and specific heat capacity of the composite material along and perpendicular to the fiber direction are as follows, where 1 and 2 represent, respectively, the two directions parallel to and perpendicular to the fiber and \( l \) and \( g \) indicate the two states of curing degree of 0 and fully cured.

(a) Thermal conductivity
\[ \lambda_i = (1 - \alpha)\lambda_i^l + \alpha\lambda_i^g, \quad i = 1, 2. \]

(17)

(b) Thermal expansion coefficient
\[ \beta_i = (1 - \alpha)\beta_i^l + \alpha\beta_i^g, \quad i = 1, 2. \]

(18)

(c) Specific heat capacity
\[ C_p = (1 - \alpha)C_p^l + \alphaC_p^g. \]

(19)

The mechanical properties of the T300 fiber are shown in Table 3.
The elastic modulus and Poisson ratio of the cured resin are shown in Table 4.

During the molding process, the elastic modulus of the resin is greatly affected by the degree of curing and less affected by temperature. The change process of the elastic modulus of the resin is shown in the following formula [21]:

$$E_m = E_m^0 (a < \alpha_{gel}),$$

$$E_m = (1 - \alpha_{mod}) E_m^0 + \alpha_{mod} E_m^\infty (a \geq \alpha_{gel}),$$

where $\alpha_{gel}$ is the gel point of the resin, generally around 0.4 [14], the value in this article is 0.38, and the relevant parameters of the uncured system are shown in Table 5.

In the finite element simulation calculation process, the curing process parameters are consistent with the parameters of the mold temperature field calculated in the previous chapter. The boundary conditions imposed by the simulation are as follows: the temperature node data of the molding profile is derived through CFD-POST. While ensuring that the coordinates of the lower surface of the wall plate are consistent with the upper surface, the temperature load is given to the wall plate in the form of node temperature. At the same time, the upper surface of the component is covered by the auxiliary material, and the convective heat exchange with the hot air is carried out. The convective heat transfer coefficient of the upper surface and the side surface of the component is set to $20 \text{Wm}^{-2}\text{K}^{-1}$ [22]. When calculating the model, the fixed time increment step is set to 50 s.

When calculating the cure-induced deformation of the composite panel after molding, static-general analysis is used to create two analysis steps. The first step is to calculate the stress and strain during the curing process of the component, and the component is in the unreleased state in the process, and the second step is to calculate after the mold is released. In the first step of the calculation process, first, add the boundary conditions to the component. Since the thermal expansion performance of the mold material is close to that of the component, the mold and the component are not considered. The stress between the components fixes and restrains the component profile that fits the molding profile; the upper surface of the component is covered by the pressure field in the tank during the molding process, and the excess resin is discharged from the side, so the upper surface of the component is applied 0.6 Mpa pressure load. In the second step of the stress release process, change the restraint method to fix the 4 nodes at the center of the member, so that the material will undergo stress release in this state.

3.5. Calculation Results. Figure 10 shows the final curing deformation result of the composite panel member. After the stress is released, the component bends upwards and a rebound occurs. The maximum deformation of the component is 8.182 mm. The deformation is mainly caused by the anisotropy of the material properties and the unevenly distributed temperature field. These factors cause the component to produce an inward bending moment and finally, spring back deformation.

In order to study the effect of mold temperature distribution on the deformation of the component, this paper analyzes the cure-induced deformation of the composite panel under a uniform temperature field. When calculating the temperature field, the temperature load on the lower surface of the component is set to be consistent with the curing process curve, and the entire area is evenly distributed. The calculation result is shown in Figure 11.

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**Table 2: The parameters used in the curing kinetics model.**

| Heating rate (°C/min) | 1       | 3       |
|-----------------------|---------|---------|
| $A_1 \times 10^5$ s$^{-1}$ | 6.913   | 6.997   |
| $A_2 \times 10^5$ s$^{-1}$ | 3.175   | 3.380   |
| $M$                   | 0.648   | 0.633   |
| $n_1$                | 2.885   | 2.926   |
| $n_2$                | 0.821   | 0.769   |

**Table 3: Mechanical property of T300.**

| Property          | Value |
|-------------------|-------|
| $E_1$ (GPa)       | 152.669 |
| $E_2$ (GPa)       | 8.435  |
| $\nu_{12}$        | 0.2476 |
| $E_{m0}$ (GPa)    | 3.483  |
| $\nu_{m0}$        | 0.336  |

**Table 4: Mechanical properties of composite and cured resin.**

| Property          | Value |
|-------------------|-------|
| $E_m^0$ (GPa)     | 233   |
| $E_m^\infty$ (GPa) | 8.435 |
| $\nu_{m}^0$       | 0.2476 |
| $E_{m0}$ (GPa)    | 3.483  |
| $\nu_{m0}$        | 0.336  |

**Table 5: Mechanical property of uncured resin.**

| Property          | Value |
|-------------------|-------|
| $E_{m0}$ (MPa)    | 20.8  |
| $K_m^0$ (GPa)     | 1.416 |
| $\nu_{m}^0$       | 0.4975 |
| $G_{m0}$ (MPa)    | 6.944 |
| $\alpha_{gel}$    | 0.38  |

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**Figure 9: Geometrical model of the panel.**
It can be seen from the analysis that the maximum cure-induced deformation of the composite panel calculated under a uniform temperature field is 3.619 mm, which is also bent upward. In summary, the uneven temperature field
During the molding process of the autoclave will cause the cure-induced deformation of the composite panel components to increase. For this reason, it is necessary to study the performance changes during the molding process of the components.

The temperature and the degree of cure change of different parts of the component during the molding process are analyzed. It is consistent with the above-mentioned method of analyzing the temperature field of the mold surface. Three nodes uniformly distributed along the diagonal line of the siding component were chosen. The temperature and curing degree data are derived and plotted in Figure 12.

During the curing process, due to the small thickness of the composite panel, the temperatures of the selected three nodes are basically the same as the above-mentioned temperature load applied. The temperature of the node near the tank door rises the fastest, and the temperature of the center node rises the slowest. There is a large temperature difference during curing. When the temperature is close to the holding temperature, the curing rate increases rapidly, so the temperature gradient of the component makes the curing rate not synchronized in different areas. It can also be seen from the figure that the curing degree of the node near the tank door rises fastest, the final curing degree reaches 0.899, the curing degree of the central node rises the slowest, and the final curing degree is 0.877. The maximum curing degree difference reached 0.22939, which would cause differences in the internal performance of the components. In turn, the cure-induced deformation of the component is increased, and the molding accuracy of the component is reduced.

According to the calculation results of the model proposed in this paper, a composite mold with ventilation holes is manufactured, as shown in Figure 13. The cure-induced deformation of the composite panel manufactured by this mold was characterized by placing the composite part on the manufactured mold and measuring the four points (depicted in Figure 11) from the part perpendicular to the mold. The cure-induced deformations are 3.34 mm, 2.41 mm, 3.34 mm, and 2.38 mm for \( A_1 \), \( A_2 \), \( A_3 \), and \( A_4 \), respectively. The measurements show good agreement with the simulated results, verifying the accuracy and effectiveness of the numerical method proposed in the present study. It also illustrates the importance of using numerical simulation methods to calculate the mold temperature field and the cure-induced deformation of components to guide the actual engineering.

4. Conclusion

In this paper, the temperature field of the large-scale frame mold in the autoclave forming process and its effect on the cure-induced deformation of the component is studied. Firstly, a temperature field calculation model is established; then the mold temperature field results obtained are used as the temperature load in the curing process. The cure-induced deformation calculation model of the component is established to predict the deformation of the component after demolding.

It can be seen from the results that the component cure-induced deformation is increased by as much as 2 times when the calculated temperature field load is applied, compared with the uniform temperature load. This is due to the large temperature gradient generated on the surface of the large frame-type mold during the molding process, which makes the cure induced of the components asynchronous. Therefore, temperature uniformity has a great influence on the forming performance of large-scale components, and it is necessary to optimize the design during the manufacturing process. The mold temperature field and component cure-induced deformation model established in this paper can effectively guide mold designers to optimize the design of frame molds in the actual manufacturing process.

Data Availability

The raw/processed data required to reproduce these findings cannot be shared at this time as the data also forms part of an ongoing study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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