Cure Simulation for Composite Materials Using OpenFOAM

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Cure kinetics plays a critical role in the determination of the practical performance of polymeric composite materials. Because such materials are widely used in aerospace and automobile applications, simulation and optimization of the cure cycle are valuable and desirable for economic sake.

In the cure process, heat is required to initialize the polymerization which is exothermic and thermally activated. Therefore, the local temperature and degree of cure determine the instantaneous local reaction rate. As in previous research [1-3], the compression molding of a polyester sheet molding compound (SMC) is modeled by diffusion reaction system equation:

$$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T + \rho H_i \frac{\partial \alpha}{\partial t}$$ ....(1)

where \(\rho\) and \(c\) are the density and the specific heat of the composite material, \(k\) is the thermal conductivity. And, the second term on the right hand side is the rate of heat generation, where \(H_i\) is the total heat of reaction, which can be determined by differential scanning calorimetry (DSC), and \(\alpha\), the degree of cure ranging from 0 to 1. We adopt the model of cure kinetics used by [4], detailed information is provided as Equations.2 and the cure parameters as Table 1.

$$\frac{\partial \alpha}{\partial t} = f(\alpha, T)$$

$$= \left(a_1 e^{-d_1/RT} + a_2 e^{-d_2/RT} \alpha^n \right)(1-\alpha)^n$$ ....(2)

A different method [2,5], Finite Element Method, was previously employed to simulate this behavior, which also provide quantitative and comparable way to verify the validity of the method described in this study.

In this study, original LaplacianFOAM solver is modified accordingly to employ cure simulation. A 1D Studied case is quantitatively reestablished by using the same initial and boundary conditions from reference [2] as Equations 3-5. And resultant plots as cure degree and temperature profiles are shown, compared to references [2, 3], and analyzed as Figure 1, 2.

Initial condition and boundary conditions:

\[ T(z,0) = T_0(z), \quad 0 \leq z \leq h \ldots (3) \]

\[ T(h,t) = T_h(t), \quad 0 \leq t \leq \tau \ldots (4) \]

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\[ T'(0,t) = 0, \quad 0 \leq t \leq \tau \ldots \ldots (5) \]

where, \( h \) is the half of laminate thickness, and \( \tau \) the simulation time.

<table>
<thead>
<tr>
<th>Material Properties</th>
<th>( \rho = 1900 \text{kg.m}^{-3} )</th>
<th>( a_1 = 4.9 \times 10^{14} \text{sec}^{-1} )</th>
<th>( m = 1.3 )</th>
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<tbody>
<tr>
<td></td>
<td>( c = 1.0 \text{J.g}^{-1}.\text{K}^{-1} )</td>
<td>( a_2 = 6.2 \times 10^{5} \text{sec}^{-1} )</td>
<td>( n = 2.7 )</td>
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<tr>
<td></td>
<td>( k = 0.53 \text{W.m}^{-1}.\text{K}^{-1} )</td>
<td>( Hr = 84 \text{J.g}^{-1} )</td>
<td>( d_1 = 140 \text{kJ.mole}^{-1} )</td>
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<td></td>
<td></td>
<td>( d_2 = 51 \text{kJ.mole}^{-1} )</td>
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Table 1 Material Properties

The OpenFOAM model agrees quantitatively with the finite difference (FD) model, but only qualitatively with the finite element method (FEM) model at reference [5]. We are working to understand the discrepancy.

REFERENCES


