

Finite Element Modeling of Composite Hydrogen Cylinders in Localized Flame Impingements

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ABSTRACT

The objective of this paper is to develop a comprehensive non-linear finite element model for determining failure behavior of hydrogen composite storage cylinders subjected to high pressure and flame impingements. A resin decomposition model is implemented to predict the residual resin content. A material degradation model is used to account for the loss of moduli. A failure model based on Hashin's failure theory is implemented to detect various types of composite failure. These sub-models are implemented in ABAQUS finite element code using user subroutine. Numerical results are presented for thermal damage, residual properties and resin content.

INTRODUCTION

Composite cylinders are typically made of carbon-reinforced epoxy resins and usually designed to bear very high pressures of 5,000 – 10,000 psi. Due to the high pressure and flammable nature of the polymer resins, the stiffness reduction and the growing fire via the polymer matrix material will result in a catastrophic failure when subjected to fire. It is therefore necessary to study the fire response of high pressure composite cylinders for their safe operation.

Many investigations have been conducted by various researches [1-3] on the behavior of high pressure composite cylinder under mechanical loadings. Using finite element method, numerous studies have been performed on high-pressure cylinder analysis [4-6]. Different one-dimensional thermal models have been developed to predict the temperature and the residual resin content through the thickness as a function of time [7-10]. These models account for heat transfer by conduction, resin decomposition, and the cooling effect of volatile products passing through the laminate. However, compared to pure mechanical loading and

pure thermal loading, there have been few studies on the fire response analysis of high-pressure composite cylinder subjected to the combined thermal and mechanical loads [11-12].

In this paper, a coupled thermo-mechanical dynamic finite element model has been developed to simulate the composite hydrogen cylinder subjected to high pressure and heat flux on the wall surface. The model is formulated in an axisymmetric coordinate system which accounts for out-of-plane stresses and reduces computational cost dramatically. When the polymer materials are exposed to a sufficiently high temperature (200-300°C), decomposition reactions and thermo-chemical expansion begin to occur and the resin system degrades to form gaseous products and carbonaceous char. In order to incorporate this phenomenon, the thermal model is built to account for gas convection and heat generation of decomposition in addition to conduction of the composite, convection and radiation of surface. The fire source is modeled as a constant heat flux throughout the simulation. Inner pressure of the cylinder is dependent on temperature of hydrogen gas which is modeled as a sink temperature. The sink temperature is updated based on the amount of heat absorbed by hydrogen gas from the inner surface of cylinder. The variation of material properties with temperature is significant for composites, especially at high temperatures. A temperature dependent material model has been developed and implemented. Hashin's theory is used as progressive failure criterion to predict different types of failure (matrix cracking and fiber breakage). All the models are developed and implemented in commercial finite element code ABAQUS, using user subroutines. A typical high pressure composite hydrogen cylinder is simulated using the developed model and results related to safety concerns for cylinder on fire are reported.

MODELING FOR HIGH PRESSURE COMPOSITE HYDROGEN CYLINDERS

A strong sequentially coupled thermal-stress approach is implemented in predicting the behavior of composite hydrogen cylinder subjected to flame impingements and internal high pressure. At each increment, the temperature profile is obtained using the thermal and resin reaction models. The temperature field is then imported to the mechanical model with material damage information from previous increment. The pressure of the inner cylinder is updated based on the heat absorption of hydrogen gas, which is computed from temperature profile. The thermal and mechanical models are solved sequentially in each increment. As the wall consists of a large number of laminae, modeling each lamina will cause extraordinary computational cost, especially when thermal and damage models are also incorporated. Hence, a homogenization technique is used to smear several laminae to a sub-laminate as in Figure 1. The equivalent moduli of the sub-laminate are used in the formulation of finite element model.

THERMAL MODEL

The high temperature will cause the resin decomposition of the cylinder composite wall. The decomposition rate of the resin is usually represented by Arrhenius's law and can be expressed as:

$$\frac{\partial \rho}{\partial t} = -A \rho \exp(-E_A / RT) \quad (1)$$

where, ρ – density,
 t – time
 T – temperature
 A – pre-exponential factor
 E_A – activation energy
 R – gas constant

Material constants A and E_A are determined using Differential Scanning Calorimetry.

With the consideration of resin reaction, the heat transfer equilibrium equation has to include resin decomposition energy and vaporous migration energy. As the dimension of thickness direction is much less than those of hoop and axial directions, the vaporous gas are only assumed to transfer in thickness direction. The axisymmetric heat diffusion equation can be written as:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial r} \left(k_r \frac{\partial T}{\partial r} \right) + \frac{1}{r} \left(k_r \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial T}{\partial z} \right) + \dot{m}_g C_{pg} \frac{\partial T}{\partial r} + \frac{\partial \rho}{\partial t} (Q - h_{com} - h_g) \quad (2)$$

where, C_p – specific heat of composite
 k – thermal conductivity
 r – displacement through the thickness

$\dot{m}_g$ – gas mass flux
 C_{pg} – specific heat of gas
 Q – heat of decomposition

If the accumulation of the generated gas is ignored, the gas mass flux at any spatial location can be calculated as:

$$\dot{m}_g = \int_{t_w}^{r_h} \left(\frac{\partial \rho}{\partial t} \right) dr_h \quad (3)$$

where, r_h – distance from hot face
 t_w – wall thickness of composite

SUB-LAMINATE MODEL

The principle of sub-laminate (Figure 1) homogenization is based on the assumption that the in-plane strains and the interlaminar stresses through the thickness are constant [13-16].

The lamina stress-strain relationship in global coordinate can be written as:

$$\begin{Bmatrix} \langle \sigma_o \rangle \\ \sigma_i \end{Bmatrix} = \begin{bmatrix} C_{oo} & C_{oi} \\ C'_{oi} & C_{ii} \end{bmatrix} \begin{Bmatrix} \varepsilon_o \\ \langle \varepsilon_i \rangle \end{Bmatrix} \quad (4)$$

where, C_{oo} , C_{oi} and C_{ii} are sub matrices of global stiffness matrix. $\langle \sigma_o \rangle$ and σ_i are out-of-plane and in-plane stresses respectively. ε_o and $\langle \varepsilon_i \rangle$ are out-of-plane and in-plane strains respectively. $\langle \rangle$ represents the term is constant through laminate.

Partially inverting Eq. (4) yields

$$\begin{Bmatrix} \varepsilon_o \\ \sigma_i \end{Bmatrix} = \begin{bmatrix} C_{oo}^{-1} & -C_{oo}^{-1}C_{oi} \\ C'_{oi}C_{oo}^{-1} & -C'_{oi}C_{oo}^{-1}C_{oi} + C_{ii} \end{bmatrix} \begin{Bmatrix} \langle \sigma_o \rangle \\ \langle \varepsilon_i \rangle \end{Bmatrix} \quad (5)$$

After averaging, Eq. (5) can be expressed as

$$\begin{Bmatrix} \langle \varepsilon_o \rangle \\ \langle \sigma_i \rangle \end{Bmatrix} = \begin{bmatrix} A & -B \\ B^T & D \end{bmatrix} \begin{Bmatrix} \langle \sigma_o \rangle \\ \langle \varepsilon_i \rangle \end{Bmatrix} \quad (6)$$

where, $A = \sum_{k=1}^N \frac{t_k}{t} (C_{oo}^{-1})_k$, $B = \sum_{k=1}^N \frac{t_k}{t} (C_{oo}^{-1}C_{oi})_k$,

$$D = \sum_{k=1}^N \frac{t_k}{t} (-C'_{oi}C_{oo}^{-1}C_{oi} + C_{ii})_k$$

t_k is the thickness of each lamina in the smeared sub-laminate and t is the total thickness of the smeared sub-laminate.

Partially inverting Eq. (6) yields the equivalent stiffness matrix Q_{eq} of the sub-laminate as

$$\begin{Bmatrix} \langle \sigma_o \rangle \\ \langle \sigma_i \rangle \end{Bmatrix} = \begin{bmatrix} A^{-1} & A^{-1}B \\ B^T A^{-1} & B^T A^{-1}B + D \end{bmatrix} \begin{Bmatrix} \langle \varepsilon_o \rangle \\ \langle \varepsilon_i \rangle \end{Bmatrix} \quad (7)$$

The equivalent compliance matrix (for angle-ply laminate) is given by

$$[Q_{eq}]^{-1} = \begin{bmatrix} A^{-1} & A^{-1}B \\ B^T A^{-1} & B^T A^{-1}B + D \end{bmatrix}^{-1} = [S_{ij}] \quad (8)$$

Equivalent engineering properties used for the simulation can be obtained from Eq. (8) as

$$\begin{aligned} E_{11} &= 1/S_{44}, \quad E_{22} = 1/S_{55}, \quad E_{33} = 1/S_{11} \\ G_{12} &= 1/S_{66}, \quad G_{13} = 1/S_{33}, \quad G_{23} = 1/S_{22} \\ \nu_{12} &= -S_{45}/S_{44}, \quad \nu_{13} = -S_{14}/S_{44}, \quad \nu_{23} = -S_{15}/S_{55} \end{aligned} \quad (9)$$

After the global stresses and strains of sub-laminates are obtained, the stresses in each lamina are obtained in the global material coordinates by

$$\begin{aligned} (\sigma_o)_k &= \langle \sigma_o \rangle \\ (\sigma_i)_k &= (B^T)_k \cdot \langle \sigma_o \rangle + (D)_k \cdot \langle \varepsilon_i \rangle \end{aligned} \quad (10)$$

where, k is the k^{th} lamina of the sub-laminate.

Finally, the stresses in local material coordinate system can be obtained by standard coordinate transformation.

FORMULATION OF FINITE ELEMENT MODEL

Axisymmetric formulation for transient analysis can be written as

$$[M^e]\{\ddot{\Delta}^e\} + [K^e]\{\Delta^e\} = \{F^e\} + \{F_T^e\} \quad (11)$$

where, $[M^e] = 2\pi \int_s \rho [N]^T [N] r ds$,

$$[K^e] = 2\pi \int_s [B]^T [C] [B] r ds$$

$$\{\Delta^e\} = \{\{u_r\} \{u_\theta\} \{u_z\}\}^T$$

$\{F^e\}$ and $\{F_T^e\}$ are forces due to mechanical and thermal loads respectively. In addition, N is interpolation function, B is strain displacement function, C is elasticity matrix, ρ is density and (u_r, u_θ, u_z) are displacement components in cylindrical coordinate system.

By discretizing Eq. (2), the heat conduction formulation can be expressed as

$$[C_T]\{\dot{T}\} + [K_T]\{T\} = \{H_T\} \quad (12)$$

where,

$$\begin{aligned} [C_T] &= \int_V \rho C_p N^T NdV, \quad [K_T] = \int_V N^T \cdot \underline{k} \cdot NdV \\ [H_T] &= \int_S N^T \cdot q_s dS + \int_V N^T \cdot q_r dV \end{aligned}$$

where, $\underline{k}$ is thermal conductivity, q is surface heat flux and q_r is the reaction heat due to the resin decomposition and vaporous migration.

The reaction heat q_r can be expressed as

$$q_r = \dot{m}_g C_{pg} \frac{\Delta T}{\Delta r} + \frac{\Delta \rho}{\Delta t} (Q + (C_{pg} - C_p) \cdot (T - T_\infty)) \quad (13)$$

where, C_{pg} is the specific heat of gas, T_∞ is ambient temperature and Q is heat of decomposition.

Combining Eq. (11) and (12), the sequentially coupled thermal-stress equation can be written as

$$\begin{aligned} \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}^e \begin{Bmatrix} \ddot{\Delta} \\ 0 \end{Bmatrix}^e + \begin{bmatrix} 0 & 0 \\ 0 & C_T \end{bmatrix}^e \begin{Bmatrix} \dot{\Delta} \\ T \end{Bmatrix}^e + \begin{bmatrix} K & 0 \\ 0 & K_T \end{bmatrix}^e \begin{Bmatrix} \Delta \\ T \end{Bmatrix}^e \\ = \begin{Bmatrix} \{F\} + \{F_T\} \\ \{H_T\} \end{Bmatrix}^e \end{aligned} \quad (14)$$

MATERIAL MODELS

Temperature dependent material properties

Mechanical and thermal properties of fiber reinforced composites vary significantly with temperature. As the carbon/epoxy laminate carries the pressure loading from the hydrogen gas, the effect of temperature on its material properties can not be ignored. However, the full required data of temperature dependent properties are not available in literature. Assumptions and curve fittings are necessary to obtain the material property data based on limited experimental data that is available. Numerous studies have been done on the curve fitting of temperature dependent properties. Gibson et al. [17] shows that a hyperbolic tan (tanh) function is capable of giving excellent fit to experimental data of material moduli and strength. The equation can be expressed as

$$P(T) = \left[\frac{P_U + P_R}{2} - \frac{P_U - P_R}{2} \tanh(k(T - T_g)) \right] \cdot C \quad (15)$$

where, $P(T)$ is temperature dependent material property, P_U is the unrelaxed (low temperature) value of that property, P_R is the relaxed (high temperature) value of that property, k is a constant describing the breadth of the distribution, T is temperature, T_g is the mechanically

determined glass transition temperature and C is a constant.

The experimental data of carbon/epoxy are taken from literatures [18, 19]. Moduli are fitted using Eq. (14). The curves fitting parameters are listed in Table 1. The thermal properties of carbon/epoxy are listed in Table 2 and Table 3. Properties for resin reaction model are listed in Table 4.

The strength of the composite is dependent on temperature and resin content. It has been assumed that the temperature variation of the ultimate longitudinal, transverse and shear strengths of carbon/epoxy follow the same pattern as that as the longitudinal, transverse and shear moduli respectively and resin content only affects the transverse and shear strengths. The virgin strength used this investigation is listed in Table 5.

Composite failure criteria

As the composite wall of the hydrogen cylinder experiences combined mechanical and thermal loads, a variety of failure types would occur in the process. A progressive failure model is employed in this study to identify the failure types based on failure criterion and predict the safety state of the cylinder. Hashin's failure criterion [20], accounting for four possible modes of ply failure, is used for this purpose.

1. Matrix tensile or shear cracking ($\sigma_{22} + \sigma_{33} \geq 0$)

$$I_{mt} = \frac{(\sigma_{22} + \sigma_{33})^2}{(F_T^t)^2} + \frac{\sigma_{12}^2 + \sigma_{13}^2 + \sigma_{23}^2 - \sigma_{22}\sigma_{33}}{(F_{LT}^s)^2} \quad (16)$$

2. Matrix compressive or shear cracking ($\sigma_{22} + \sigma_{33} < 0$)

$$I_{mc} = \frac{1}{F_T^c} \left[\left(\frac{F_T^c}{2(F_{LT}^s)} \right)^2 - 1 \right] (\sigma_{22} + \sigma_{33}) + \frac{(\sigma_{22} + \sigma_{33})^2}{4(F_{LT}^s)^2} + \frac{\sigma_{12}^2 + \sigma_{13}^2 + \sigma_{23}^2 - \sigma_{22}\sigma_{33}}{(F_{LT}^s)^2} \quad (17)$$

3. Fiber tensile fracture ($\sigma_{11} \geq 0$)

$$I_{ft} = \left(\frac{\sigma_{11}}{F_L^t} \right)^2 + \frac{1}{(F_{LT}^s)^2} (\sigma_{12}^2 + \sigma_{13}^2) \quad (18)$$

4. Fiber compressive fracture ($\sigma_{11} < 0$)

$$I_{fc} = - \left(\frac{\sigma_{11}}{F_L^c} \right) \quad (19)$$

where, F_L^t , F_L^c , F_T^t , F_T^c and F_{LT}^s are longitudinal tensile strength, longitudinal compressive strength, transverse tensile strength, transverse compressive strength and shear strength of unidirectional ply respectively.

Once a specific type of failure is identified in the laminate, the reduction in its load-carrying capacity is accounted for by a reduction in its elastic moduli based on Tan's [21] assumption: (a) When matrix tensile or shear cracking occurs, properties (E_{22} , G_{12} , G_{23}) are taken as 0.2 times original values. (b) When matrix compressive or shear cracking occurs, properties (E_{22} , G_{12} , G_{23}) are taken as 0.4 times the original values. (c) When fiber tensile fracture occurs, E_1 is taken as 0.07 original values. (d) When fiber compressive fracture occurs, E_{11} is taken as 0.14 times the original values.

Model for hydrogen gas

The hydrogen gas in the cylinder absorbs energy and increases the internal pressure. In the present study, the hydrogen gas effect is modeled as a sink whose temperature is updated at each increment based on the amount of heat flux going through the inner cylinder surface. The internal pressure of cylinder is computed from the state equation of hydrogen. The experimental data of hydrogen gas is taken from literature [22]. The pressure and temperature relationship at constant density (23.59 kg/m³, when temperature is 20°C and pressure is 34.5 MPa) is curve fitted as shown in Figure 2. The fitted equation is employed to compute cylinder internal pressure.

CYLINDER DESIGN

The cylinder design used in present study is taken from Mitlitsky et al. [23]. Netting analysis is used to determine the thickness of cylinder wall. The parameters are summarized in Table 6.

FINITE ELEMENT ANALYSIS

An axisymmetric finite element model is built in ABAQUS as shown in Figure 3. The length of cylinder part is taken as $L_c = 0.3$ for analysis and the dome curve follows the geodesic path. The flame source is modeled as a constant heat flux (75 KW/m²) applied on the area with length L_s through out the analysis. The radiation, as well as the convection, is also considered at the cylinder outside surface. Pressure is imposed on the inner liner surface. A symmetric boundary condition is applied at the end of cylinder to reduce the model to half of the cylinder. The model uses SAX8RT element accounting for both deformation and heat transfer. The cylinder wall consists of inner aluminum liner and six sublaminae of carbon/epoxy (Figure 4). Each hoop (90°) and helical (±10°) sub-laminate consists of many laminae.