Multiscale modeling of damage and fracture of a composite overwrapped pressure vessel

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Abstract. An approach to multiscale modeling of damage and fracture of a composite overwrapped pressure vessel based on experimental studies is presented. The proposed approach takes into account the interaction of mechanical properties and structural parameters of the composite material at each scale level and their joint interaction. A micromodel of the fracture of a composite material has been developed taking into account the structural features. Calculated mechanical and strength properties of unidirectional composite material are determined. A mesomodel of fracture of a layered composite material is presented for numerical three-point flexural tests. Experimental verification of the numerical mesomodel of straining and fracture of a layered composite material has been carried out. A comparative analysis of the experimental data and numerical modeling showed the quantitative and qualitative agreement of the results. A macromodel of damage and fracture of a composite overwrapped pressure vessel is presented. The diagrams of progressive damage in a composite shell depending on the mode of fracture are presented. An assessment of the strength of the vessel structure is given taking into account the initiation and evolution of damage in the composite shell.

1. Introduction
The design of a composite overwrapped pressure vessel (COPV) consists of a VT1-0 sealing titanium liner and a 9-layer composite shell based on IMS60 carbon fibers and an ED-1 epoxy matrix. Modeling the fracture of structures using composite materials (CM) made by filament winding is a complex task.

Straining and fracture of a layered composite shell is a multi-stage process that covers various scale levels [1-6], where each level is interrelated and affects the general characteristics of mechanical properties. Three scale levels are considered: microlevel, mesolevel and macrolevel. When CM is subjected to mechanical loads, various fracture processes occur within all three scales simultaneously.

Analysis of literature sources led to the conclusion that in the development multiscale numerical models, the relationship with experimental studies is not always traced. In numerical simulation of fracture of a COPV, simplified models are used, which do not take into account the elastic plastic properties of the liner and contact. In addition, there are not many authors who take into account the design and technological features of CM and their influence on the stress-strain state of the COPV.

In this regard, for a better understanding of the behavior the straining and fracture of the COPV, it becomes necessary to development numerical models that take into account the processes of fracture at each scale level. The aim of this work was to development multiscale model of the fracture of a
COPV taking into account the design and technological features of CM. To achieve this goal, several tasks were solved:

- development of a micromodel of fracture of CM to determine the mechanical properties and ultimate strengths depending on the type of loading;
- experimental verification of the calculated mechanical and strength properties on the numerical mesomodel of fracture of a layered CM;
- development of a macromodel of damage and fracture of a COPV for studying the processes of straining and fracture depending on the applied pressure.

2. Micromodel of composite material fracture

In the CM mechanics, systems of joint interaction of structural elements are considered, taking into account micromechanical effects on the “fibers-matrix” scale [7]. Such models make it possible to predict effective mechanical properties, inhomogeneous stress and strain fields, and also to simulate the fracture of CM as a multistage process.

Using the ANSYS Mechanical APDL finite element analysis, a 3D numerical micromodel of CM was developed, which includes a number of features: generation of random arrangement of carbon fibers inside the matrix; modeling of random distribution of mechanical properties; modeling fracture of structural elements.

Based on the studies in [8], the fibers in the CM are located randomly and even with large distances between them, which makes it necessary to model a variant with a random arrangement of fibers inside matrix. In addition, most carbon fiber-reinforced CM have a high variation of mechanical properties [9]. The coefficient of variation of the Young’s modulus is 0.22, and for the ultimate tensile strength is 0.25. The model of the scatter of mechanical properties is based on the division of each fiber into sectors with different values of mechanical properties, which are described according to the normal distribution.

The fracture of structural elements of the CM is modeled by reducing the stiffness matrix of the elements by the degradation coefficient $D = 1 \times 10^{-6}$. At each stage of loading, an analysis of stresses in the elements is carried out, if the element does not fulfill the strength condition, then it fracture. In these studies, the criterion of maximum stress was used depending on the type of loading.

A numerical micromodel of a unidirectional CM with a chaotic arrangement of fibers, in which the fiber and matrix are isotropic materials is presented in figure 1. Geometrical parameters of the model: carbon fiber percentage $V_f = 70\%$, fiber diameter $d_f = 5 \mu m$, fiber length $L = 650 \mu m$, side of a square $B = 30 \mu m$.

![Figure 1](image)

**Figure 1.** Numerical micromodel of fracture of a unidirectional CM: (a) tensile design scheme; (b, c) finite element of model of structural elements of CM.

Mechanical and strength properties of structural elements in CM are presented in table 1.
Table 1. Mechanical and strength properties of structural elements CM.

| Characteristic          | Carbon fiber IMS60 | Epoxy resin ED-1 |
|-------------------------|--------------------|------------------|
| Young’s modulus, MPa    | 290000             | 3000             |
| Tensile strength, MPa   | 5800               | 50               |
| Poisson’s ratio         | 0.28               | 0.32             |

On the basis of the developed micromodel, a multivariate numerical experiments of CM were carried out and the main of mechanical properties and ultimate stress values were determined depending on the type of loading: under tension ($X_t$) and compression ($X_c$) along the direction of reinforcement; under tension ($Y_t$) and compression ($Y_c$) across the direction of reinforcement; shear ($S_l$). The fracture process of CM under the action of a tensile load in the direction of the reinforcement is presented in figure 2.

![Fractured fiber](image)

Figure 2. Numerical micromodel of fracture of a unidirectional CM: (a) strain curve of CM under tension; (b) fiber fracture simulation process.

The calculated mechanical and strength properties CM are presented in table 2 and 3.
Table 2. Mechanical properties CM.

| Characteristic | $E_1$, MPa | $E_2 = E_3$, MPa | $\nu_{12} = \nu_{13}$ | $\nu_{23}$ | $G_{12} = G_{13}$, MPa | $G_{23}$, MPa |
|---------------|------------|------------------|---------------------|-------|-------------------|--------|
| Value         | 129000     | 5800             | 0.32                | 0.45  | 3400              | 3800   |

Table 3. Ultimate strength properties CM.

| Characteristic | $X_1$, MPa | $X_2$, MPa | $Y_1$, MPa | $Y_2$, MPa | $S_1$, MPa |
|---------------|------------|------------|------------|------------|------------|
| Value         | 2334       | -969       | 50         | -100       | 50         |

Thus, the calculated values of mechanical properties and ultimate strengths were determined with a known set of data on each structural element of the CM.

3. Mesomodel of fracture of a laminated composite material

The mesomodel consists of a package of differently oriented composite tapes. Continuum damage model (CDM) was used to simulate fracture at the meso and macro levels. The model is based on a continuous process of degradation of the mechanical properties of the material due to the accumulation of damage [10]. Material degradation spreads throughout the model according to the failure criteria as long as the structure is able to redistribute the load. This causes to the use of CDM at the meso and macro scales, since at the microlevel, fracture is modeled by a sharp decrease in the stiffness matrix of the element and its exclusion from the calculation, which in turn not allow correctly displaying the process of straining and fracture of the CM.

To predict progressive damage using CDM, it is necessary to determine 8 parameters: 4 values of energy dissipated per unit area depending on the fracture mode; 4 viscous damping coefficients depending on the fracture mode.

Energy dissipated per unit area is determined by the equation:

$$G_e = \frac{u_{eq}^f}{\int_0^{u_{eq}} \sigma_{eq} \, du_{eq}} = \frac{1}{2} \sigma_{eq}^f u_{eq}^f,$$

(1)

where $\sigma_{eq}, u_{eq}$ – equivalent stress and displacement, respectively; $\sigma_{eq}^f, u_{eq}^f$ – ultimate equivalent stress and displacement, respectively.

Using equation (1) and the results obtained at the microlevel, the energy presented in table 4 was calculated.

Table 4. Energies parameters of CM.

| Characteristic | $G_e^{X1}$, N·mm$^{-1}$ | $G_e^{X2}$, N·mm$^{-1}$ | $G_e^{Y1}$, N·mm$^{-1}$ | $G_e^{Y2}$, N·mm$^{-1}$ |
|---------------|-----------------|-----------------|-----------------|-----------------|
| Value         | 23.34           | 5.82            | 0.325           | 0.7             |

Viscous damping coefficients for the various modes were taken from the [11] and presented in table 5.

Table 5. Energies parameters of CM.

| Characteristic | $\zeta_e^f$ | $\zeta_e^l$ | $\zeta_e^m$ | $\zeta_e^m$ |
|---------------|-------------|-------------|-------------|-------------|
| Value         | $1 \cdot 10^{-3}$ | $1 \cdot 10^{-3}$ | $5 \cdot 10^{-3}$ | $1 \cdot 10^{-3}$ |

The initiation of damage is determined using failure criterion. In these studies, the Hashin failure criterion [12] was used to determine the mods of fracture. Damage parameter $d$ for each type of
fracture is calculated by equivalent displacements. Damage variables increase gradually based on the energy amounts dissipated for the various damage modes:

\[ d = 1 - \frac{u_{eq}^0 (u_{eq}^0 - u_{eq})}{u_{eq} (u_{eq}^0 - u_{eq})}, \]  

(2)

where \( u_{eq}^0 \) – equivalent displacements corresponding to initiation of fracture.

Due to the initiation of damage in the material, the stiffness in the elements decreases. The damaged elastic matrix is defined as follows:

\[
[C]_d = \frac{1}{A} \begin{bmatrix}
(1 - d_f)E_f & (1 - d_f)(1 - d_m)v_{12}E_f & 0 \\
(1 - d_f)(1 - d_m)v_{12}E_f & (1 - d_m)E_m & 0 \\
0 & 0 & A(1 - d_f)G
\end{bmatrix},
\]

(3)

where \( A = 1 - v_{12}v_{21}(1 - d_f)(1 - d_m); \) \( E_f, E_m, G \) – undamaged elastic and shear modulus; \( d_f, d_m, d_s \) – damage parameters depending on the mode of fracture.

Experimental verification of the numerical mesomodel of straining and fracture of a layered CM has been carried out. Plane specimens of a 9-layer CM were modeled at various reinforcement angles relative to the central axis (0, 45 and 90 degrees) for numerical three-point flexural tests (figure 3). The model used mechanical properties and ultimate strength values calculated on the micromodel.

Average geometric dimensions of specimens and models: number of layers \( n = 9; \) layered thickness \( h_{ply} = 0.34 \text{ mm}; \) thickness \( h = 3.06 \text{ mm}; \) width \( b = 20 \text{ mm}. \) Radius of curvature for different reinforcement angles: \( R_0 = 506 \text{ mm}; \) \( R_{45} = 504 \text{ mm}; \) \( R_{90} = 236 \text{ mm}. \)

![Figure 3](image-url)  

**Figure 3.** Design scheme (a) and finite element model (b) for three-pint flexural test.

Based on the results of the numerical modeling of the CM for three-point flexural tests, “load-deflection” diagrams were constructed for each specimen (figure 4).
Comparative analysis of experimental data [8] and numerical modeling showed the qualitative and quantitative correspondence of the straining and fracture process of specimens with different reinforcement angles. The considered numerical model, which is determined by the mechanical and strength properties of the CM, as well as damage and fracture modeling using CDM, is applicable for COPV modeling and allows to reliably estimate its strength.

4. Macromodel of the fracture of a composite overwrapped pressure vessel

In most cases, the analysis of the stress-strain state of the COPV is performed using axisymmetric finite elements or three-dimensional elements of a layered shell [13, 14]. Initially, the cross-section of the liner and the composite shell was determined on the basis of theoretical relations for calculating the thickness [15], and then a volumetric model of the repeating sector was built by rotating around the axis. Due to the technological features of winding the composite tape on the liner, the thickness of the composite shell is not constant, it continuously increases from the equator to the pole hole. Composite shell formed by two-zone filament winding.

COPV geometrical dimensions: shell radius $R = 506$ mm; shell height from equator $Z = 281$ mm; pole hole radius $r_1 = 35$ mm and zone of “hump” radius $r_2 = 95$ mm. The design scheme and finite element model are presented in figure 5.
The mechanical properties of elastic-plastic titanium VT1-0 are presented in table 6.

**Table 6. Mechanical properties of titanium liner.**

| Characteristics | $E$, MPa | $\mu$ | $\sigma_{\text{yield}}$, MPa | $\sigma_{\text{US}}$, MPa |
|-----------------|----------|-------|-----------------------------|--------------------------|
| Value           | 110000   | 0.32  | 380                         | 430                      |

The pressure was applied to the inner surface of the liner with a constant increase in value. The contact between the liner and the composite shell was set with a friction coefficient of 0.2.

Based on the performed numerical calculations, the curves of equivalent strains of the structural elements of the COPV were constructed, taking into account the initiation and evolution of damage in the composite shell (figure 6). Based on the figure, it can be seen that the structure loses its bearing capacity at a pressure of 20.25 MPa.

![Figure 5](image-url)
Figure 6. Curves of equivalent strains of structural elements of COPV (a) and the distribution of total damage in the composite shell at a pressure of 17.5 MPa (b).

The distribution of damage in the composite shell under different modes of fracture is presented in figure 7. The distribution of damage at $P/P_{\text{max}} = 0.4$ corresponds to the initiation of damage in the composite shell, and $P/P_{\text{max}} = 1$ to its end. Damage level is rated in the range from 0 (intact element) to 1 (fractured element).
Figure 7. Distribution of damage depending on the position of the radius $r$ of the composite shell: (a) matrix tension; (b) matrix shear; (c) fiber tension; (d) matrix compression.
Due to the lower strength of the CM in the transverse direction, damage to the matrix initially occurs in the area of pole hole and the “hump” zone (figure 7 (a)). As the load increases, damage grows along the direction of the equator. In addition, shear damage to the matrix occurs in the layers (figure 7 (b)), resulting in tensile damage in the carbon fibers (figure 7 (c)). The initiation of damages in the fibers during compression is not observed, and in the matrix, they are insignificant (figure 7 (d)). The circumstance is explained by the fact that behavior of the composite tape upon application of internal pressure is close to stress state of a unidirectional CM under tension along the direction of reinforcement.

When high damage occurs in the CM, extensive plastic strains occur in the liner in the area of the flange. In this area, a high concentration of local strains is observed, caused by a change in the stiffness of the material due to an increase in the thickness of the flange in comparison with the bottom membrane. Parallel to this, the stiffness in the layers is significantly reduced, which leads to a loss of the COPV load-bearing capacity.

Under the action of internal pressure in the COPV, several stages of deformation and destruction can be distinguished: elastic straining of the CM; elastic-plastic straining of the liner; initiation and evolution of damage in the CM; liner critical straining; local fracture of the composite shell and liner; loss of the COPV load-bearing capacity.

5. Conclusions
An approach to multiscale modeling of a composite overwrapped pressure vessel based on experimental studies is presented. Developed multilevel models of fracture of CM taking into account design and technological features.

A micromodel of CM fracture is presented, taking into account random structural features. The proposed model allows one to determine the effective mechanical and strength properties with a known set of data on the structural elements of CM.

An experimental verification of the obtained mechanical and strength properties, as well as parameters characterizing damage and fracture at the meso and macro levels, has been carried out. Comparative analysis showed qualitative and quantitative agreement of the results.

The COPV micromodel has been developed, which takes into account the technological and design features of the CM. Using the CDM, the developed numerical model allows for reliable tracking of straining processes, as well as damage and fracture in the composite shell. The determined limiting pressure for the considered configuration of the COPV, which is 20.25 MPa.

Thus, the developed combined approach makes it possible to track the processes of straining and fracture of CM at each scale level, and to assess the strength of the COPV at design stage.

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