Multiphysics Multiscale Simulation Platform for Damage, Environmental Degradation and Life Prediction of CMCs in Extreme Environments

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**Project Summary**

**Methodologies**
- Experiments
- Multiscale CMC Characterization
- Thermomechanical Tests

**Experiments**
- UD Frame

**Multiscale CMC Characterization**
- Damage Hotspots

**Stochastic Multiscale Framework**
- Low Cost & High-Fidelity Solvers

**Modeling**
- Temperature Effects

**Objectives**
- Develop a stochastic concurrent multiscale framework for accurate analysis of CMC components operating in turbine service environments
- Integrate modeling and experiments
- Incorporate developed models into life prediction methodologies and FEA software for more accurate estimate of service life

**Schedule**

<table>
<thead>
<tr>
<th>BP2</th>
<th>BP3</th>
<th>BP1</th>
</tr>
</thead>
<tbody>
<tr>
<td>10/1/10-9/30/19</td>
<td>10/1/20-9/30/21</td>
<td>10/1/21-8/15/22</td>
</tr>
<tr>
<td>Qtr1</td>
<td>Qtr2</td>
<td>Qtr3</td>
</tr>
</tbody>
</table>

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- Jacob Schichtel – NDSEG fellow, no cost to the grant
- Dr. Luke Borkowski (RTRC) – Major Participant
Overview

▪ Key Issues & Objectives
▪ Tasks & Technical Framework
▪ Research Progress
  - Material Characterization & Uncertainty Quantification
  - Thermomechanical Progressive Damage Modeling
  - Creep Modeling
  - Damage-diffusion Oxidation Coupling
  - Integrated Multiscale Framework
▪ Publications
▪ Concluding Remarks & Future Work
▪ Acknowledgements
Key Issues & Objectives

- Next generation CMCs must meet challenges of DOE’s advanced turbine concepts, which involve inlet temperatures up to 3100°F, high thermal gradients, multi-regimmed oxidation & mechanical loading over long time periods
- Limited knowledge of CMC response and damage in operating environment
- Significant manufacturing induced flaws and scale-dependent architectural variability
- Temperature-dependent damage mechanisms & failure modes
- Matrix progressive damage creates pathways for gaseous oxidants to attack CMC interior; distinct effects in intermediate & high temperature
- Interface and load sharing between constituents strongly influences material behavior

Enhance the understanding of CMC degradation & failure in service conditions through more accurate life prediction methodologies - reduce empiricism & enable improved utilization of CMCs in turbine applications
Integrated Multiscale Framework

High-fidelity Multiscale Generalized Method of Cells – concurrent/synergistic analysis of complex fiber architectures, normal shear coupling

MSGMC - Liu & Chattopadhyay, 2011
Task 1: Project Management and Planning

Task 2: Material Characterization & Uncertainty Quantification
- Multiscale CMC Characterization
- Uncertainty Quantification
- Stochastic Microstructural Simulation

Task 3: Multiphysics Constitutive Modeling
- Thermomechanical Progressive Damage
- Creep-Fatigue (Dwell Fatigue)
- Fiber-Matrix Interface
- Environmental Degradation & Oxidation

Task 4: Integrated Multiscale Framework
- Concurrent Multiscale Framework
- Multiscale HFGMC

Task 5: Integration into an FEA Model

Task 6: Testing & Validation
- Thermomechanical Testing
- Analysis of Damage Mechanisms
- Thermogravimetric Testing

Develop more Accurate Life Prediction Methodologies and Integrate with FEA Software
Material Characterization and Uncertainty Quantification

Motivation: Systematically factor uncertainty into the model and capture effects of length-scale dependent variability on CMC response

- Material characterization
- Uncertainty assessment
- Stochastic microstructural simulation & RVEs

3D Statistical characterization and material variability

3D high-fidelity microscale model

- Microscale response
  - Matrix cracking
  - Fiber failure
  - Intra-tow matrix porosity

Composite Weave

3D mesoscale model

- Mesoscale response
  - Tow/matrix debonding
  - Crossover defects

Material/architectural stochasticity

Model Input

Model Input

Model Input
Material Characterization

- Characterization, quantification, & representation of multiscale material & architectural variabilities
  - Inter-tow porosity volume fraction
  - Intra-tow porosity volume fraction
  - Fiber volume fraction
  - Fiber radii
  - Inter-tow spacing
  - Intra-tow spacing
  - Tow size & shape

- Image processing algorithms for material feature recognition & image segmentation

- Information used in multiscale analysis
S200H confocal microscopy results

Confocal microscopy allows more accurate quantification of intratow architectural features over X-ray uCT; micrographs will facilitate construction of microscale S200H SRVEs (Task 2.3)
a: shrinkage crack between different ceramic phases (ceramics particles and SiNC matrix)

*b: different ceramic phases in intratow regions

c: fiber hexagonal close packing

d: intratow porosity

Multiple phases detected in matrix regions; preferable fiber packing structure & intra-tow porosity identified; fiber/matrix interphase layer not visible
High-resolution macroscale tomographs show SiC/SiNC versus C/SiNC geometry, internal structure & architectural variability in as-received material.
Intertow regions have higher oxidation volume fractions than intratow regions; carbon-rich interphase layer observed around fibers.
C/SiNC CMC Variability

Image processing algorithm developed to detect multiscale structural & defects variability

Scanning electron micrograph of intra-tow region

Segmented grayscale image

Fiber cross sections & intra-tow defects

- Porosity volume fractions: Intra-tow ~3%; Inter-tow: ~5%
- Tow cross section: 1498.221µm x 172.673µm
- Fiber radius: 2.4846 µm (mean); standard deviation 0.1489 µm
- Fiber volume fraction: 49.59%

Image processing algorithms under development to generate detailed 3D stochastic representative volume elements (SRVEs). Micrographs illustrating intra-tow matrix porosity. Microscale SRVEs containing intra-tow matrix porosity.

Accurate in-situ microstructural representation will facilitate accurate modeling of damage initiation, progression, & subsequent failure.
Image processing algorithms currently under development to generate detailed 3D stochastic representative volume elements (SRVEs) will facilitate accurate in-situ microstructural representation. Accurate in-situ microstructural representation will facilitate accurate modeling of damage initiation, progression, & subsequent failure.
- 400 SRVEs generated with 1-3% intra-tow porosity VF
- Elastic properties obtained using high fidelity micromechanics theory

Presence of intra-tow matrix porosity deteriorates elastic properties of UD C/SiNC CMC. Larger standard deviation in transverse & shear
Converted high-fidelity SRVEs to finite element (FE) based grids

Geometry for single fiber from the developed generator & FE-based geometry
Microstructural Simulation & SRVE

von-Mises & shear stress comparison

Structured grid (SRVE generator)

Structured mesh (ABAQUS geometry)

Good agreement with results from FE geometry and ABAQUS
Incorporated SRVEs in parallelized HFGMC (pHFGMC)

Transverse stresses & strains comparison

Good agreement between FE and pHFGMC solvers
Multiscale analysis uses localization & homogenization schemes to bridge the length scales - **key issue is the size of the RVE over which homogenization is conducted**

- Stochastic RVE (SRVE): RVE in the presence of disorder/stochasticity in the microstructure
- A minimum SRVE size is required to approximate the mesoscale material behavior
- Minimum SRVE size increases
  - As stochasticity increases*
  - Critical for simulating nonlinear mechanical behaviors (plasticity, damage, failure)**

Characteristic lengths
- \( d \): Microscale (e.g., fiber diameter)
- \( L \): SRVE
- \( L_{meso} \): Mesoscale

Weak stochasticity \( d \ll L \ll L_{meso} \)

Large stochasticity \( d \ll L \ll L_{meso} \)

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**Example: SRVE for Tow Failure**

- Unknown SRVE size for tow failure

Experimentally observed tow behavior:
- **I**: Linear elastic behavior
- **II**: Nonlinear behavior with matrix cracking until saturation
- **III**: Nonlinear behavior with sequential fiber failure

Model assumptions:
- No fiber failure occurs in region II
- Matrix has no load sharing role in region III
- Stochasticity arises from varying fiber strengths

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**Stochasticity in tow failure behavior due to varying fiber strengths**

*Chateau (2014); **Calard, V., & Lamon, J. (2004)*
SRVE for Tow Failure

- Force controlled loading until failure
- Fiber strengths randomly sampled from experimental Weibull distribution
- Global load sharing is assumed

Tow strength prediction strongly depends on number of fibers - illustrates importance of minimum SRVE size

Increase in number of fibers decreases stochasticity
SRVE for Tow Failure: Modified Fiber Damage Model

- Objective: Simulate strength of tows with 500 fibers using an equivalent 20-fiber SRVE
- Each fiber consists of 25 pseudo fibers with the same cross-sectional area & initial elastic stiffness

Experimental Weibull distribution of strength for Hi-Nicalon fiber *

- Fiber failure model modified to a discrete-progressive damage model
- If the stress on a fiber exceeds the strength of one of its pseudo fibers, then that pseudo fiber fails:
  - Fiber stiffness degraded accordingly
  - Strengths of remaining pseudo fibers degraded by the same fraction

The modified fiber damage model enables the SRVE to capture stochasticity in tow fiber failure strength with significantly reduced number of fibers.

- Tow strength distributions with the 20-fiber SRVE compare well with 500-fiber tows.
- Stress-strain responses show excellent agreement.

The modified fiber damage model enables the SRVE to capture stochasticity in tow fiber failure strength with significantly reduced number of fibers.
Bayesian framework for uncertainty assessment

Model input parameters: $\theta$

Prior estimates of the parameters: $P(\theta)$

The probability of observations $X_{obs}$ given the parameters ($\theta$) and uncertainty: $P(X_{obs}|\theta)$

Multiscale model (Task 3)

Observations: $X_{obs}$

Experimental testing (Task 6)

Bayesian inference

$P(\theta|X_{obs}) \propto P(\theta)P(X_{obs}|\theta)$

Updated probability distributions of the parameters: $P(\theta|X_{obs})$

Bayesian inference for estimating parameters of material behavior models based on sparse characterization data & experimental observations
Thermomechanical progressive damage model accounting for crack growth & nucleation and micropore formation

- Incorporation of flaw statistics, temperature dependent material properties
- Crack & void growth governed by fracture mechanics, crack growth kinetics
- Matrix cracks activate when stress intensity factor exceeds critical value; crack growth rate affected by temperature, environment

\[
\sigma_{ij} = (1 - D)C_{ijkl}(\varepsilon_{kl}^{tot} - \varepsilon_{kl}^{p} - \varepsilon_{kl}^{D} - \varepsilon_{kl}^{T})
\]

\[
\dot{D} = \begin{cases} 
\dot{D}_{p} & K_I \leq K_{IC} \\
\dot{D}_{c} & K_I > K_{IC} 
\end{cases}
\]

- \(C\): Elastic stiffness tensor
- \(\varepsilon^{tot}\): Total strain
- \(\varepsilon^{p}\): Porosity-based strain
- \(\varepsilon^{D}\): Flaw growth-based strain
- \(\varepsilon^{T}\): Thermal strain
- \(D\): Damage ISV
- \(D_{p}\): Porosity ISV
- \(D_{c}\): Matrix cracking ISV
- \(K_I\): Stress intensity factor (SIF)
- \(K_{IC}\): Critical SIF

Skinner and Chattopadhyay (2020) Composite Structures
Cooldown Framework

- CMC response highly dependent on as-produced thermal residual stress and damage state
- Developed multiscale cooldown simulation framework to determine thermal residual stress at micro-, meso-, and macroscales in CMC weave
- Applied temperature-dependent damage model with cooldown framework to capture manufacturing-induced damage and residual stresses

**Thermal Residual Stresses**

2D Woven C/SiC (5HS weave architecture)

Cooldown framework captures realistic initial state with thermal residual stress profiles, initial damage distribution
Cooldown Framework

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Thermal Residual Stresses

Cooldown framework captures realistic initial state with thermal residual stress profiles, initial damage distribution. Damage initiates in undulating tows and propagates to the intertow matrix subcells.
Results
- Cooldown framework captures realistic initial state, accounts for manufacturing-induced damage, thermal residual stresses
- Mechanical loading simulation captures nonlinear elastic material behavior, first matrix cracking

**Comparison with Experiment**

Loading direction: Longitudinal

Cooldown simulation followed by mechanical loading simulation makes framework applicable to entire range of CMC operating temperatures
Creep Modeling

Complex creep behavior in CMC components, under sustained loading & elevated service temperatures, occurs across multiple length scales and interacts with the inherent brittle damage behavior of the individual constituents.

**Accurate CMC component life prediction requires in-depth understanding of creep, creep-fatigue, and damage interactions across the length scales**

**Key Issues**

- Time-dependent constituent load transfer due to differing creep rates; CMC creep consists of creep & relaxation in constituents
- Damage mechanisms & failure modes depend on constituent creep susceptibility
- Thermal residual stresses in as-produced CMC parts affect subsequent creep behavior

Develop a 3D viscoplasticity model; integrate into a micromechanics framework to simulate constituent creep & subsequent time-dependent load transfer

Creep Modeling

Development of 3D thermomechanical orthotropic viscoplasticity model
- Norton-Bailey creep power law
- Hill orthotropic plastic potential
- Arrhenius temperature dependence
- Associative flow rule
- Time-hardening and strain-hardening formulations

- Matrix damage modeled with previously developed thermomechanical progressive damage model (Task 3.1)
- Curtin progressive damage model applied to simulate stiffness reduction due to successive fiber failure

Constitutive law:
\[ \sigma_{ij} = (1 - D) C_{ijkl} (\varepsilon_{kl}^{tot} - \varepsilon_{kl}^{I} - \varepsilon_{kl}^{th}) \]
where \( \varepsilon_{ij}^{I} = \int_0^t \dot{\varepsilon}_{ij} dt \) and \( D = \int_0^t \dot{D} dt \)

Constituent model parameters will be determined from in-house creep-fatigue tests
Creep Modeling

3D orthotropic viscoplasticity formulation incorporated into generalized method of cells (GMC) micromechanics framework

- Effective stiffness matrix

\[ \bar{C} = \frac{1}{h_{tot}l_{tot}} \sum_{\beta=1}^{N} \sum_{\gamma=1}^{N} C^{(\beta,\gamma)} A^{(\beta,\gamma)} h_{\beta} l_{\gamma} \]

- Global RUC stresses

\[ \bar{\sigma} = \frac{1}{h_{tot}l_{tot}} \sum_{\beta=1}^{N} \sum_{\gamma=1}^{N} \sigma^{(\beta,\gamma)} h_{\beta} l_{\gamma} \]

\( A \): Strain concentration tensor
\( h_{\beta}, l_{\gamma} \): Subcell dimensions
\( h_{tot}, l_{tot} \): RUC dimensions
\( N_{\beta}, N_{\gamma} \): Number of subcells in each dimension

Unidirectional GMC RUC

GMC integration facilitates simulation of CMCs with arbitrary microstructures & ply/weave architectures; enables simulation of creep in individual constituents & associated constituent load transfer
Thermal residual stress effects, Contd.

- Simulated response – Hi Nicalon SiC/CVD-SiC microcomposite subjected to thermal cooldown from 1450 °C to RT followed by 100 MPa creep at 1000 °C

Constituent stresses in load direction vs. time

- Post-manufacturing cooldown causes as-produced tensile stress in matrix & compressive stress in fiber (matrix CTE > fiber CTE)
- Creep causes redistribution of constituent residual stresses; matrix creeps first and sheds load to fiber; matrix is in compression and fibers are in tension upon unloading

* Model calibrated using microcomposite creep test results presented in Rugg et al. (1999)
Higher predicted inelastic (creep) strain for higher processing temperature due to process-induced compressive stress in matrix, which is less creep-resistant than fiber for the SiC/SiC microcomposite.

* Plotted strain is $\varepsilon_{11}^{total} - \varepsilon_{11}^{thermal}$
Creep-damage Modeling

Simulated total longitudinal strain time history for Hi-Nicalon/CVD-SiC CMC single fiber microcomposite

- Prescribed loading: 381 MPa (constant), 1300 °C
- Matrix damage simulated with developed thermomechanical progressive damage model
- Fiber damage & failure simulated with Curtin progressive damage model

Incorporation of matrix and fiber progressive damage models permit simulation of i) tertiary creep; ii) microcomposite progressive damage; iii) microcomposite failure

* Rugg et al. (1999).
Creep-damage Modeling

Simulated constituent stress and strain time history for Hi-Nicalon/CVD-SiC CMC single fiber microcomposite

- Prescribed loading: 381 MPa (constant), 1300 °C

Incorporation of matrix and fiber progressive damage models permit simulation of:

i) tertiary creep; ii) microcomposite progressive damage; iii) microcomposite failure
Oxidation plays a major role in the response of CMCs at elevated temperatures

- Matrix cracks create passages for oxygen to diffuse into the material
- Oxidation of the fiber interphase or the fusion of the SiC fiber to the SiNC matrix impairs load transfer capabilities
- Oxidation reaction of oxygen-exposed SiNC matrix activates at extreme temperatures, resulting in a multi-regimed response


Model under development to address complex coupling between anisotropic damage, diffusion, crack closure, & oxidation of the fiber-matrix interphase at the microscale
Model under development

- Anisotropic damage model with crack closure
- Nonlinear damage-diffusion coupling
- Oxidation model - couple concentrations of gaseous oxygen to interface material
- User defined elements (UELs) with additional concentration degrees of freedom developed & integrated into Abaqus FE software

Oxidation of Fiber Interface

Need for Computational Efficiency

Necessary to balance fidelity & efficiency to enable model scalability

- Multiscale handshaking methods: Hierarchical, concurrent, synergistic
- Hierarchical models unable to admit constitutive nonlinearity; precludes simulation of creep & progressive damage
- Concurrent models prohibitively computationally expensive
- Part & component simulation require parallelization & model order reduction

Additional efficiency required in presence of:

- Complex geometry
- Multiple analysis scales
- Material & geometric uncertainty
- Time-dependent nonlinear material behavior

Approach: Increase computational efficiency & model scalability via parallelization & model order reduction techniques
Need for Computational Efficiency

- GMC*: First-order local fields – highly efficient; lack of normal-shear coupling & local field gradients*
- Higher order local fields necessary to accurately model nonlinear response and failure
- HFGMC***: Second-order local fields – highly accurate; admits normal-shear coupling & local field gradients

*GMC: Generalized Method of Cells; **Aboudi et al., (2012) ***HFGMC: High Fidelity Generalized Method of Cells

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**Improved fidelity of HFGMC comes at significant computational cost**
**Efficient HFGMC implementation necessary for model scalability**
Efficiency Improvement

Methodology to achieve computational efficiency

- Most memory & time-consuming operation in HFGMC is inversion of global stiffness matrix
- Global stiffness matrix must be computed every time local subvolume experiences damage
- Multiscale simulations require solution of multiple expensive micromechanics simulations at every time increment

Combination of efficient reformulation, sparse matrix representation & parallel processing used to achieve improved computational efficiency

Illustration of sparsity in global stiffness matrix & methodology used to achieve computational efficiency

Efficiency Improvement

HFGMC computational performance results

- Computation time and memory savings increase when larger subcell configurations are simulated
- Additional time savings achieved using parallel processing

- Improved HFGMC efficiency through use of sparse matrices & parallelization techniques
- Memory required and computation time reduced by two orders of magnitude

Efficient HFGMC Implementation – Verification

Benchmark problem*

Unidirectional composite RUC

In-plane shear strain

- HFGMC second order displacement field captures normal-shear coupling
- Local stress fields in agreement with reference values
- Current HFGMC implementation performs better, i.e. closer to FEM, than reference HFGMC* at boundaries

Results compare well with benchmark problem; verifies efficient HFGMC implementation

Incorporation of Plasticity and Thermal Effects in HFGMC

Test case for thermal strains

- CTE = -0.0005
- $\Delta T = 10$
- Effective unit cell strain, $\varepsilon = 0$
- Negligible stiffness in directions 2 & 3

Results

$\varepsilon_1 = -0.0025$

$\varepsilon_1 = 0.0025$

Test case for plastic strains

- Negligible stiffness
- CTE = 0
- E = 200 GPa; $\nu = 0.17$
- $Y_0$ (initial yield stress) = 8 MPa
- $h$ (hardening coefficient) = 2 GPa

Results

Expected linear strain hardening behavior recovered

The methodology will allow accurate analysis of processing-induced thermal residual stresses, creep & damage
HFGMC (elastic case) has been implemented into Abaqus as a user-defined material subroutine for implicit (UMAT) and explicit (VUMAT) FEA in Abaqus.

- VUMAT/UMAT will be extended to include inelastic and thermal effects.

**Inputs**
- Material constituent properties
- Fiber/Void/Interphase volume fractions and arrangement
- Fiber orientation

**Results**

**Microscale**
- HFGMC UMAT will facilitate simulation of realistic coupon/part geometries & boundary conditions while accounting for microstructural architectural features.
Background and Motivation

- *High-fidelity multiscale* simulation of CMCs requires solution of *multiple* scale-dependent SRVEs
- Woven CMC architecture requires at least two analysis scales
- Efficient handshaking & structural scale integration requires additional computational efficiency

Model order reduction necessary to enable i) efficient handshaking across multiple scales; ii) integration of developed tools into continuum-scale life prediction tools
Approach

Machine learning (ML)-based reduced order model (ROM) to improve computational efficiency & facilitate structural scale integration; enforcement of governing physical laws & constraints will guide inference & ensure physical consistency & model stability

- Replace effective nonlinear constitutive law of microscale SRVEs with ML-based reduced order model (ROM)
- Use of custom layers to endow NN architecture with domain-specific knowledge to i) guide model inference; ii) satisfy physical laws & constraints
- Custom layers will solve constrained convex optimization problems to enforce physical consistency; optimization problem solved within layer need not have closed form solution

Challenge – learned constitutive law must be thermodynamically consistent; numerical integration requires symmetric positive definite tangent stiffness matrix
Machine Learning-based Reduced Order Model (ROM)

Schematic of ROM implementation in multiscale framework

Microscale RVE

Mesoscale RVE

Coupon tests & simulation

Task 2.1: Material Characterization

Task 6: Closed-loop testing and validation

Task 2.1: Stochastic Microstructural Simulation & RVEs

ML ROM

5HS FEM mesh (no matrix)

Task 4: Integrated Multiscale Framework

Task 5: Integration into an FEA Model

FEM coupon simulation

Initial development of ML-based ROM focused on replacing microscale SRVEs; model architecture amenable to other scales in integrated multiscale framework
Closed Loop Testing and Validation

**Experiments**
- Multiscale material characterization
- Low, intermediate & high test temperatures
- Quasi-static tensile testing
- Creep-fatigue testing in air and inert atmosphere
- Thermal properties of interest: specific heat, thermal diffusivity, CTEs

**Project Tasks**
- Material Characterization and Uncertainty Quantification
- Multiphysics Constitutive Modeling
- Integrated Multiscale Framework
- Integration into FE Model
- Testing & Validation

- Calibrate creep model parameters
- Inform/update damage model
- Identify key micro mechanisms that govern creep-fatigue
- Identify PEL change
Publications

Journals


Conferences


Concluding Remarks

Development of integrated multiscale multiphysics framework to model CMC material response under service conditions

- Characterized SiC-SiNC and C-SiNC CMCs using SEM, EDS, Micro-CT, and confocal microscopy
- Quantified uncertainty and generated detailed 3D SRVEs
- Incorporated 3D SRVE in structural scale FE simulation
- Developed cooldown framework and temperature-dependent damage model - i) simulates manufacturing-induced damage & thermal residual stresses; ii) captures nonlinear thermomechanical response
- Developed a novel 3D orthotropic creep model
- Formulated a model for the microscale oxidation of fiber interface with complex coupling between anisotropic damage, diffusion, crack closure, & oxidation
- Developed parallelized efficient pHFGMC framework; accounted for plasticity & thermal effects
- Initiated NN-based ROM development to improve computational efficiency

Future Work

- Thermomechanical testing
- Bayesian framework for UQ
- Model refinement & validation
- Oxidation model and integration with multiscale analysis
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Micrographs illustrating SiC/SiNC and C/SiNC CMC weave structure and defect types such as (i) denuded matrix, (ii) shrinkage cracks, (iii) inter- and intra-tow defects interactions, (iv) open porosity, and (v) intra-tow porosity.