A MULTISCALE MODELLING APPROACH TO GENERATE VIRTUAL TEST DATA FOR MACHINE LEARNING

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ABSTRACT

Owing to their excellent energy absorption characteristics, high-performance fiber-reinforced polymer (FRP) composites are regarded as viable candidates for use in energy absorbing structures in automobiles. However, the temperature and strain rate-dependent nonlinear deformation response coupled with variations in the multiscale structure of fabric FRP composite materials poses challenges in simulating and optimizing their properties. During the last decade, many studies demonstrated that machine learning (ML) algorithms are capable of obtaining nonlinear constitutive models for materials from complex data sets. Although data-driven ML algorithms, including artificial neural networks (ANN), have been applied in the constitutive modeling of FRP composites, their application to practical design problems is limited since there is a lack of sufficient training data. In this study, a multiscale finite element (FE) modelling approach is proposed to generate virtual stress-strain data for a unidirectional non-crimp fabric (UD-NCF) FRP composite material, with the goal of expanding the available experimental data set into large data sets for ML purposes. First, a microscopic analysis was conducted to analyze the micro and mesoscale structure of the FRP composite material. Second, coupled microscale and mesoscale FE models of the FRP material comprising manufacturing-induced defects within the representative volume elements (RVEs) were developed based on the microscopic analysis. The developed multiscale approach is intended to generate an adequate amount of reliable training and testing data for ML models based on the constituent properties and geometry of the UD-NCF FRP composites.

1 INTRODUCTION

The usage of continuous fiber-reinforced plastic (FRP) composites for load-bearing applications continues to grow at a remarkable rate since these high-performance materials exhibit excellent specific mechanical properties, including high energy absorption capabilities. However, the temperature and strain rate-dependent nonlinear deformation response and the variation of the multiscale-structure of FRP material pose challenges in simulating and optimizing their performance [1]. Until recent years, a test-and-build approach was used to tailor the material composition and mechanical properties of FRP composites and structures [2]. Virtual testing has since been utilized to predict the performance of FRP composites and reduce the extent of physical testing. Virtual testing aims to approximate the effective stress-strain response of composite materials by using the constitutive behaviors of the constituents and the material structure [3]. In this approach, a multiscale model directly connects the effective material constitutive behaviour at the macroscale to the corresponding sub-scale response (e.g., microscale and mesoscale). Thus, multiscale FE models can remove several assumptions in the constitutive laws and more accurately represent the material microstructure. However, this approach can be computationally expensive when high-fidelity simulations using three-dimensional (3D) finite element analysis (FEA) are performed [4]. For predicting the linear elastic deformation response of composite materials, several analytical and numerical studies and applications for various applications have been proposed [5, 6, 7]. To capture the nonlinear deformation response of composite materials, a multilevel finite element (FE^2) approach is widely used [8]. In the FE^2 method, the macroscale FE-based structural analysis uses effective material properties that are directly computed from microscale FE models, and additional mesoscale FE models are required for some advanced composite materials [4]. Nevertheless, the application of virtual testing has been mainly focused on quasi-statically loaded FRP composites, with limited application to predict their response under dynamic loading rates [9], which is required for structures subjected to impact loads. With the support of virtual testing tools, physics-based constitutive models have been continuously developed and improved over the years, and designated models can accurately describe the particular behaviours of composite materials. However, current physics-based constitutive models are not mature enough to accurately simulate the strain rate-dependent nonlinear deformation behaviour of the FRP composites [10, 11].

Due to the challenges of developing adequate physics-based constitutive models for FRP composites, data-driven-based constitutive models or machine learning (ML) models have recently been proposed to fill this gap, and virtual testing tools may play an important role in generating data for data-driven-based models. ML algorithms, particularly artificial neural network (ANN) models, can be used as universal estimators, which approximate complex relations between input and output data in a form-free model [12]. ANN models can learn the constitutive behaviour of FRP composites at the macroscale or the constituents' constitutive models at the sub-scale to provide a good supplement to or even replacement physics-based models. Some research works have been conducted in adopting ANN into constitutive modelling of nonlinear material behaviour of FRPs. Le et al. [13] performed a number of analyses on representative volume element (RVE) models of composite materials to generate training data for constructing a constitutive model for nonlinear elastic material behavior. Liu and co-workers [14, 15] developed various reduced order clustering surrogate models using ANN to facilitate the multiscale modeling of composite materials. Other researchers also applied different types of ANN models to construct various surrogate models to capture different nonlinear material deformation behaviors, including elasto-plasticity [16], finite deformation hyperelasticity [17] , and viscoplasticity [18]. Data-driven ML algorithms require a sizable training data set which is a major challenge since experimental data and high-fidelity multiscale simulation data are expensive and time-consuming. To construct nonlinear material models, high-dimensional input and output data are usually required. In addition, path/history-dependent materials will require additional loading history or state variables as input. Microstructural parameters (e.g., fiber architecture or microscale defects) may be also needed as additional inputs to describe the microstructure of composites. Such high-dimensional input and output data make the ANN model suffer the curse of dimensionality [19], which often requires the models to be trained with significantly larger training datasets.

The overarching aim of this study is to generate strain rate-dependent nonlinear stress-strain data for a unidirectional non-crimp fabric (UD-NCF) FRP composite material using computationally efficient multiscale FE virtual test tools, with the goal of expanding the available experimental data set into larger data sets for ML purposes. The first step of the study is presented herein, where the focus is on characterizing the microstructure of the UD-NCF FRP composite material and developing multi-scale FE models to determine the effective elastic constants. This study builds on previous work from the same research group [9].

2 MULTI-SCALE MODELLING

The concept of generating training data for a UD-NCF FRP composite material using multiscale FE virtual test tools comprises inputting selected parameter values to the FE models and obtaining the corresponding output (i.e., effective mechanical properties). Then, the relation between input and output can be determined using ML algorithms.

$$f(input\ parameters) = output\ material\ properties \tag{1}$$

To generate a large set of data, the multi-scale FE models should be able to represent the deformation behaviours of composite materials according to the inputting values while minimizing manual operations. The input parameters should cover a range of target material properties and capture the variation of material structures.

In the current study, the following steps were followed to develop multi-scale finite element models for the UD-NCF composite material:

1) Microscopic assessment of the UD-NCF composite material;
2) Characterization of the constituent materials;
3) Development of the micro-scale FE model;
4) Parametric study of the micro-scale RVE;

2.1 Microscopic assessment of the UD-NCF composite material

The investigated composite material was reinforced with the UD-NCF PX35-UD300 NCF (ZOLTEK™ Corp.), which comprised aligned tows each containing 50,000 continuous PX35 carbon fibre filaments. The tows were stitched with polyester thread in a tricot pattern and supported by transversely oriented glass fiber yarns. The matrix was a three-part snap-cure resin system, comprising EPIKOTE™ Resin TRAC 06150, EPIKURE™ Curing Agent TRAC 06150, and the mold release HELOXY™ Additive TRAC 06805 (Hexion Inc.), with a mixing ratio of 100:24:1.2 parts by weight, respectively. Flat carbon fiber/epoxy panels with a stacking sequence $[0_8]$ were fabricated using a high-pressure resin transfer molding (HP-RTM) process described in [20]. Samples with dimensions 1" x 1" were cut from the fabricated panels for optical microscopic assessment of the material structure on a cross-sectional plane perpendicular to the longitudinal direction of the fibres. The fibre volume fraction within a tow, the overall fibre volume fraction for the composite, the fibre diameter, and the geometrical parameters of the tow were measured using the image processing program ImageJ from images captured on a Keyence VHX-6000 opto-digital microscope.

2.2 Characterization of the constituent materials

The mechanical properties of the carbon fibers were taken from the study by Rouf et al. [9] (Table 1). The mechanical properties of the cured epoxy were previously characterized by Cherniaev et al. [20], and used herein (Table 2).

Table 1. Carbon fiber properties [9]

Property	Value
Longitudinal modulus (E_{11f})	242 GPa
Transverse modulus ($E_{22f} = E_{33f}$)	43 GPa
Shear modulus ($G_{12f} = G_{13f}$)	7.42 GPa
Shear modulus (G_{23f})	7.42 GPa
Poisson's ratio ($\nu_{12f} = \nu_{13f}$)	0.20
Poisson's ratio (ν_{23f})	0.49

Table 2. Cured epoxy properties [9]

Property	Value
Modulus (E_m)	2.8 GPa
Poisson's ratio (ν_m)	0.39

2.3 Development of the micro-scale finite element model

The multi-scale finite element model consisted of a micro-scale FE model and a meso-scale FE model (Fig. 1). The micro-scale FE model was used to determine the effective properties of the tow. The meso-scale FE model used the effective properties of the tow estimated by the micro-scale FE model and the matrix properties to approximate the effective properties of the UD-NCF composite (not considered herein).

A custom Python script was developed to generate the RVE for the micro-scale FE model in Abaqus 2020 Implicit based on input from the microscopic assessment of the UD-NCF composite. The important features for the micro-scale RVE included variation of fiber diameters, nonuniform fiber spatial distribution, and adjustable fiber volume fraction. The in-plane misalignment and out-of-plane crimp of the tows were not considered in the micro-scale RVE since these would be captured in the meso-scale FE model [9]. The fiber and matrix were considered to be perfectly bonded and meshed using 3D hexahedral elements. In addition, the micro-scale RVE has a periodic geometry which enabled the use of periodic boundary conditions. The effective properties of the impregnated tow were determined using well-known volume averaging techniques.

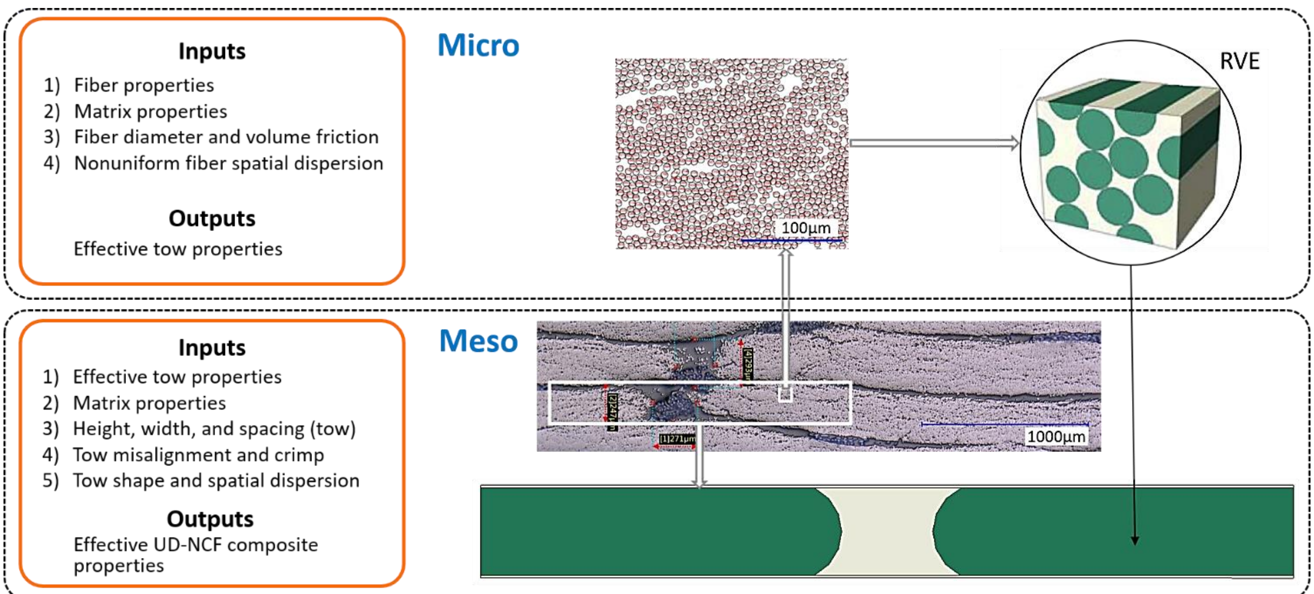

Figure 1. The connection between the micro and meso scale FE models

2.4 Parametric study of the micro-scale RVE

A parametric study was conducted to determine the influence of material and RVE parameters on the volume-averaged effective tow properties. The sensitivity of the mesh size was first studied. Next, the effect of the RVE size, which also significantly affects the simulation time, was investigated. The RVE size was identified as the ratio of RVE characteristic length to the diameter of the fibers, i.e., L/D ratio, which led to different numbers of fibers within the

RVE. Three L/D ratios (10, 15, 20) were considered, and the elastic modulus and Poisson's ratio were compared with the corresponding results calculated from the semi-empirical formulation of Chamis [21]. Finally, the fiber diameter variation for the RVE was investigated.

3 RESULTS AND DISCUSSION

3.1 Microscopic assessment of the UD-NCF composite

Obtained cross-sectional images indicated several in-tow features of the UD-NCF composite (Fig. 2). First, the carbon fibers have different diameters and are irregular in shape. The variation in fiber diameter was analyzed using ImageJ (Fig. 3). Second, many carbon fibers were compressed together because of the high-pressure manufacturing process, and some fibers were in surface contact with each other. Third, the spatial dispersion of carbon fibers was non-uniform as anticipated, and several resin-rich zones existed. Statistical analysis showed that the mean diameter of fibers in the selected area was 7.45 μm, and 95% of fiber diameters were between 6.27 μm and 8.63 μm. The fiber volume fraction of the selected area was 64.95% (Fig.3).

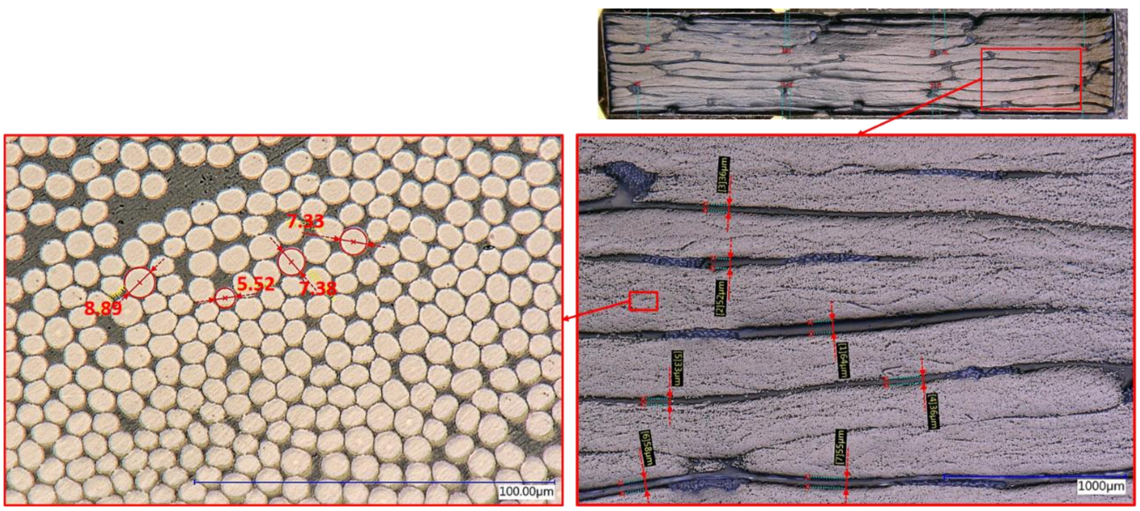

Figure 2. Cross-sectional images of the UD-NCF composite taken from an optical microscope

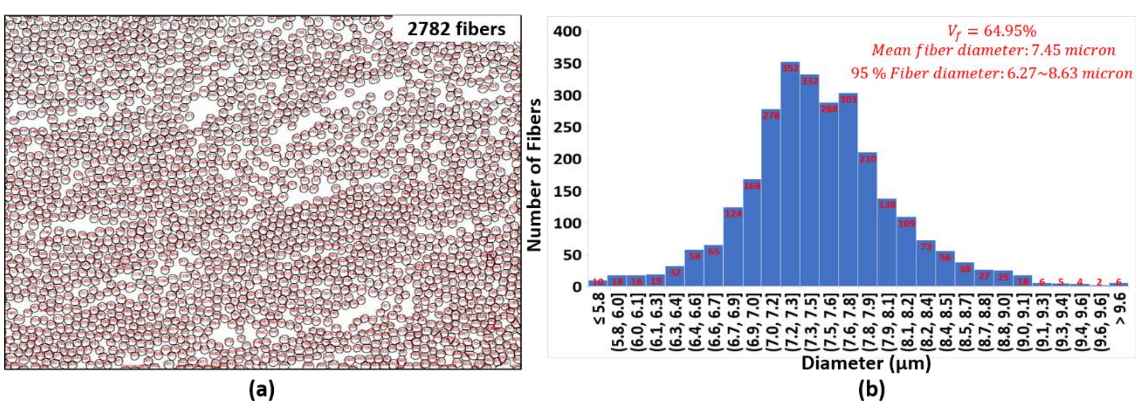

Figure 3. Statistical analysis of the variation of fiber diameters: (a) Processed image from ImageJ; (b) Statistical data of the variation of fiber diameters.

The tows were irregular ellipse shapes with significant variation in tow height and spacing. The volume fraction of the impregnated tows was estimated as 83.48%, and the features of tows were analyzed using ImageJ (Table 3).

Table 3. Geometrical features of tows

	Mean (μm)	**Standard Deviation (μm)**
Tow width	4625	106
Tow height	294	69
Vertical spacing	48	12
Horizontal spacing	275	83

3.2 Development of the multi-scale finite element model: micro-scale FE model

A statistical analysis based on a nearest neighbour distance distribution was performed for both the material and generated RVE (Fig. 4). The generated micro-scale RVE achieved an inter-fiber nearest neighbor distance distribution that is comparable with the microscopic observations of the UD-NCF FRP material.

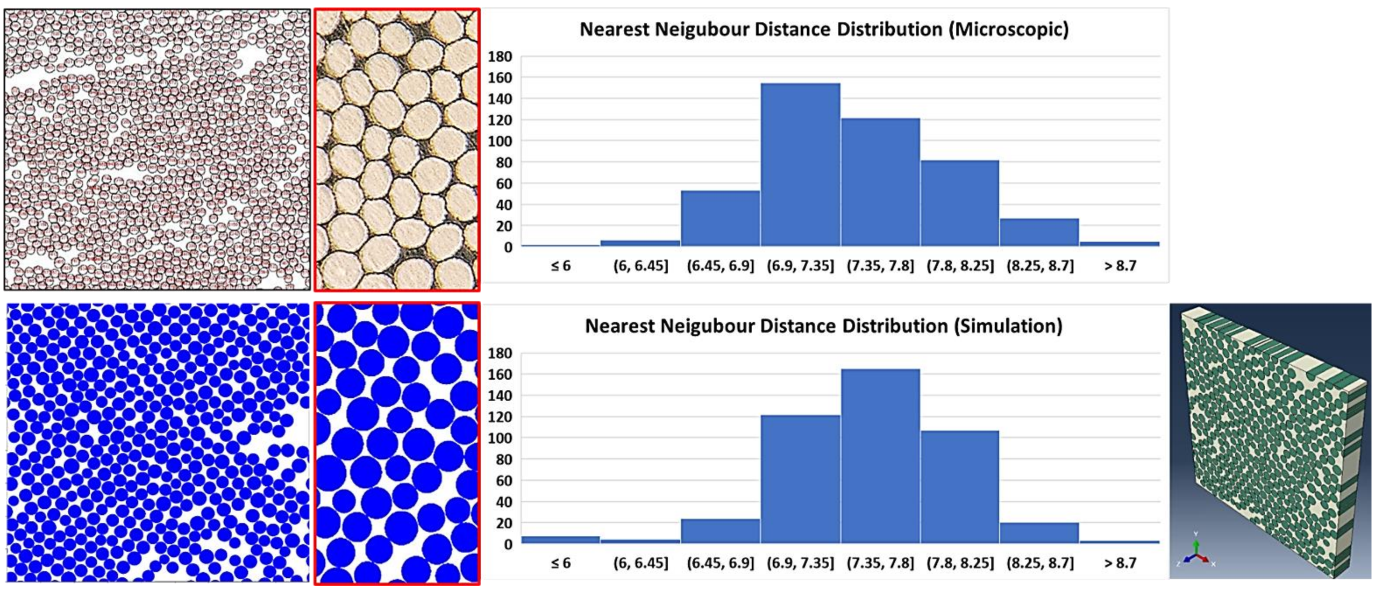

Figure 4. Fiber spatial dispersion assessment of the micro-scale RVE

3.3 Parametric study of the micro-scale finite element model

The parameters considered for the parametric study are listed in Table 4. For the mesh size sensitivity study (not shown), the global mesh size of 2, 1, 0.5, and 0.25 μm were tested, and the 0.5 μm mesh size provided a good balance between simulation time and convergence of the results. The RVE size tests showed there was no significant difference in the effective properties predicted for RVEs with different L/D ratios (Table 5), and all the predictions were closed to the results using the Chamis formulations. However, a decrease in the L/D ratio of the RVE models resulted in a notable decrease in the model simulation time. For both fiber volume fractions (V_f) cases, the effective elastic modulus of the RVE models was not significantly influenced by the feature of fiber diameter variation, while effective Poisson's ratios were slightly affected (Table 6).

Table 4. Parameters for the RVE model

Parameters		Parameters	
Fiber diameter	7, 7 ± σ* μm	V_f	50%, 60%
RVE Lengths	70, 105, 140 μm	RVE depth	10 μm
Mesh size	0.5 μm	Elements	Solid, Hex-dominated

*σ is the sample standard deviation

Table 5. Simulation results of RVEs with L/D ration of 10, 15, 20 ($V_f = 50\%$)

Properties	RVE (70x70x10)	RVE (105x105x10)	RVE (140x140x10)	Chamis formulation
$E_{11}(GPa)$	123.6	124.0	126.0	122.4
$E_{22}(GPa)$	7.79	8.05	7.97	8.26
$\nu_{12} = \nu_{13}$	0.288	0.297	0.323	0.295

Table 6. Simulation results of RVEs with/without constant fiber diameter ($V_f = 50\%, 60\%$)

RVE (70x70x10)	$E_{11}(GPa)$	$E_{22}(GPa)$	$\nu_{12} = \nu_{13}$
$V_{f,50\%}$	123.6	7.79	0.288
$V_{f,50\%}$ with Constant Ø	123.6	8.23	0.306
Chamis formulation for $V_{f,50\%}$	122.4	8.26	0.295
$V_{f,60\%}$	155.4	10.83	0.278
$V_{f,60\%}$ with Constant Ø	149.1	9.88	0.324
Chamis formulation for $V_{f,60\%}$	146.3	10.15	0.276

4 CONCLUSIONS AND FUTURE WORK

The overall goal of this study was to develop a multiscale finite element modelling approach for a unidirectional non-crimp fabric (UD-NCF) composite material to generate training data for a machine learning (ML) algorithm. The current study assessed the microstructure of the material. The key features of this material were irregular shape and inconstant diameter of carbon fibers, surface contact between carbon fibers, and non-uniform fiber dispersion. A script was developed to generate the microscale FE representative volume element (RVE) models that captured the key features of the UD-NCF composite material. The RVE models accurately predicted the effective longitudinal and transverse elastic modulus, as well as the effective Poisson's ratio. A parametric study showed the RVE length-to-fiber diameter ratio of 10 can yield good predictions in a short simulation time, while applying a constant fiber diameter to the model increased the effective Poisson's ratio values.

The future work includes developing the mesoscale RVE model, adopting nonlinear material models into the RVEs, and finally generating the high-fidelity training data for ML models.

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