

MESOSCALE MODELLING OF COMPRESSIVE RESPONSE AND DAMAGE EVOLUTION IN FLAX FIBRE REINFORCED LAMINATES

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ABSTRACT

A Modified Mesoscale Damage Theory (MMDT) was used to predict and model in-plane compressive damage behavior of natural-fiber composite, with specific parameters derived for continuous flax-fiber reinforcement. The model is developed within a thermodynamic framework and incorporates damage and inelastic evolution in the fiber direction, capturing the non-linear behaviour observed in natural fibers. The MMDT was implemented using open-source *Smart Materials Algorithms and Research Tools* (SMART+) libraries. The flax-specific parameters were derived from experimental tests and optimized with open-source algorithms. The key feature of this model, is its ability to describe the overall composite mechanical behaviour, by predicting ply-specific damage initiation, damage evolution, stiffness degradation, and inelasticity. In this paper, the proposed model successfully predicted the total strain response of E-glass/Polyester and Flax/Epoxy laminates in compression, as well as E-glass/Epoxy laminates in tension. To improve the capabilities of the proposed model, it is suggested to consider more complex shear-transverse coupling parameters, and include buckling into the constitutive equations.

1 INTRODUCTION

With continuously increasing demand for materials with high specific strength, fiber-reinforced composites have become a popular choice in major industries such as automotive and aerospace. The most popular synthetic fibers being Carbon and Glass; which have several major drawbacks including energy-intensive manufacturing, non-renewability, low degree of recyclability, and environmental damage [26]. With demand for sustainable and environmentally friendly solutions, plant-derived fibers have become a large topic of interest in contemporary composite material research. While promising fibers include hemp, jute, sisal, kenaf, and ramie; Flax has been shown to have comparable mechanical properties to Glass (Table 1), while being renewable, CO_2 neutral, recyclable, easier to process, and having a significantly smaller manufacturing and retail price compared to synthetic fibers. [2, 3, 26].

Fiber	Specific Strength (Mpa/g-cm³)	Specific Modulus (Gpa/g-cm³)	Cost per weight (\$USD/kg)	Production energy consumption (MJ/kg)
Flax	1300	20 – 70	0.5 – 1.5	11.4
Glass	1350	30	1.6 – 3.25	50

Table 1: Various properties, Flax vs Glass fibers [1]

Natural Fiber Composites (NFCs) are overlooked in engineering applications due ongoing research in the areas of flammability and operating temperatures, hydrophilic and hydrophobic properties, fiber-matrix bond strength, and non-linear mechanical behavior. Moreover, there’s a notable lack of approaches and validated methods capable of predicting internal damage initiation and evolution. Effective implementation of NFCs in mainstream industries requires a profound understanding of their damage mechanisms as well as accurate and robust predictive tools. In a recent paper, Mahboob et al. [1] has developed a Modified Mesoscale Damage Model (MMDM) for tensile loadings. It successfully accounted for the NFCs non-linear fiber-direction response, and accurately predicted flax-reinforced composite behavior under in-plane tensile loading. Experimental tests found in [28] have shown that Flax-reinforced composites under tensile and compressive loads share similar mechanical responses. Therefore, the purpose of this research was to adopt the MMDM to compressive-load cases and identify Flax-epoxy compressive- specific parameters.

2 LITERATURE REVIEW

2.1 Flax Fiber

Flax (*Linum usitatissimum*) is one of the earliest domesticated and cultivated crops; with flax fibers being used for linens as early as the Archaic period (c. 3100-2686 B.C) [4, 5]. Its unique nonlinear longitudinal behavior is rooted in its complex hierarchical structure seen in Figure 1 [6, 7]. Bast fiber bundles are composed of 10 to 40 polyhedron-shaped elementary fibers (technical fibers) surround the central (hollow) lumen, and are held together by a pectin (glue-like) interface. Elementary fibers (2 -5 cm length) seen in Figure 1b [7], are single plant cells consisting of a primary a cell wall, secondary cell wall, and lumen [8]. The bulk of the elementary fiber (circa 70%) consists of crystalline cellulose micro-fibrils located in the S2 fiber-cell layer, which spiral at a 10-degree orientation around the longitudinal axis [7-10]. There are several papers addressing Flax fiber’s tensile behavior, specifically the its stiffness variation due to microfibril re-alignment; however, significantly less papers address flax behavior under compressive loads, most focus on single fiber retting-induced defects. To the author’s knowledge, the amount of papers addressing Flax-reinforced composites behavior under compressive loads is close to none.

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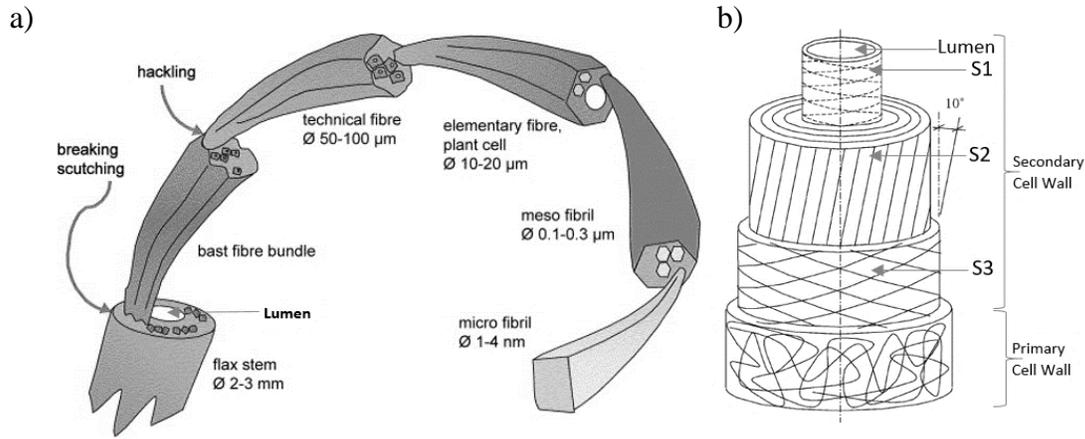


Figure 1: a) Flax stem to fiber diagram [6]; b) Elementary fiber structure [7]

2.2 Failure and Damage Theories

Damage (in the context of this paper) is referred to as local surface or volumetric discontinuities, caused by various damage mechanisms such as buckling, fiber-matrix debonding, and delamination (Figure 2). Under increasing loads, damage evolves by encouraging the development of such discontinuities, resulting in material properties degradation up to failure [20].

There are several types of theories and approaches for predicting the non-linear behavior of NFCs. Facca et al. [29] have shown that semi-empirical and polynomial-based failure criteria such as *Maximum Stress/Strain*, *Tsai-Hill*, *Tsai-Wu*, and *Hashin* can reliably predict NFC tensile modulus and strength. These models can be tailored to capture initial undamaged response, the overall laminate nonlinear behavior, and the final failure conditions. However, they cannot predict damage initiation, damage evolution, or permanent strains. The *Fracture Mechanics* approach focuses on modeling crack propagation and failure criteria due to the enlargement of set crack. This approach requires an initial crack to be present, and therefore, cannot predict damage initiation. Moreover, it focuses on a single dominant crack, and cannot simulate the complex interactions of multiple discontinuities [14,15]. Lastly, *Continuum Damage Mechanics* (CMD) techniques quantify damage and inelasticity, by representing the distribution of discontinuities via internally-evolving state variables and associated thermodynamic forces [20]. Sliseris et al. [30] proposed a CDM-based micromechanical model within a thermodynamic framework for single-ply woven Flax/epoxy composite in tension; where fiber and matrix were governed by nonlinear and isotropic hardening plasticity laws with no material properties degradation. Exercised in a finite element-based model, it successfully reproduced experimentally observed stress-strain response.

The *Mesoscale Damage Model* (MDM) developed by Ladeveze et al. [21] is a CMD-framework, shown to be a robust predictive tool for composite materials under a variety of loading conditions [20]. The prefix *Meso*, implying that the scale of analysis is in between micro (constituents level) and macro (laminate level). The key feature in this approach, is that the laminate response is predicted by separately modeling the ply and the interface; each with a constitutive law which includes damage and inelasticity. Recently, Mahboob et al. [1] accurately modeled damaged tensile mechanical response in flax laminates, by modifying the existing MDM damage evolution law in the fiber direction; effectively naming it *Modified Mesoscale Damage Model*.

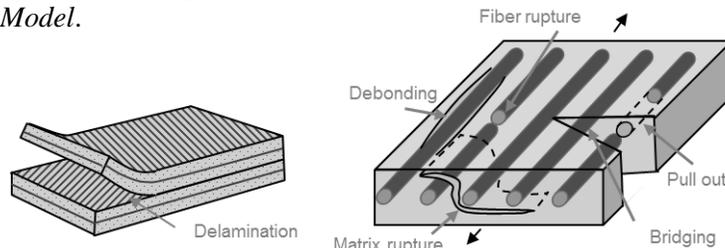


Figure 2: Failure modes of fibrous composite materials [12]

3 METHODOLOGY

3.1 Manufacturing Flax/Epoxy samples

The MMDT model requires several material parameters derived from mechanical tests. 16-layer composite plates were manufactured from unidirectional (UD) flax fabric FlaxPly® treated to an area-weight ratio of 150 g/cm². The bulk of the fabric consists of warp (0 deg) yarns held together by periodic weft (90 deg) yarns at a ratio of 40:3. Even though the material is not perfectly uniform, previous studies by Mahboob et al. [28] showed that this fabric compares well with existing data on unidirectional fabric. The matrix material is a high performance, hot curing thermoset consisting of Araldite® LY564 epoxy resin, and Aradur® 22962 hardener at a weight ratio of 4:1 respectively. A self-containing press with heating/cooling platens and programable controller was used to press and cure the composite plates according to manufacturer specifications.

3.2 Mechanical Testing

ASTM D3039 standard [17] was used to cut 250mm x 25mm x 4mm specimens from the above-mentioned plates. Composite specimens were tabbed using 64mm x 25mm x 3mm tapered Aluminum tabs, enabling fractures at the specimen mid-section. Specimens made from pure epoxy were cut into dog-bone shapes (Figure 3b) according ASRM D638 [16]. The pure epoxy specimens were used for comparison purposes.

In order to capture damage progression, repeated cycles of loading and unloading were imposed on the test specimens, with progressively increasing maximum loads up to complete failure. Figure 4a illustrates this procedure, noting that the hysteretic response is approximated as linearly elastic. Testing was conducted at room temperature and pressure, using a servo-hydraulic test frame at a displacement rate of 2 mm/min [15]. A uniaxial extensometer (0.5"-length) measured the longitudinal strain, while the transverse strain was measured by a 350Ω strain gauge; this setup is seen Figure 4b [11].

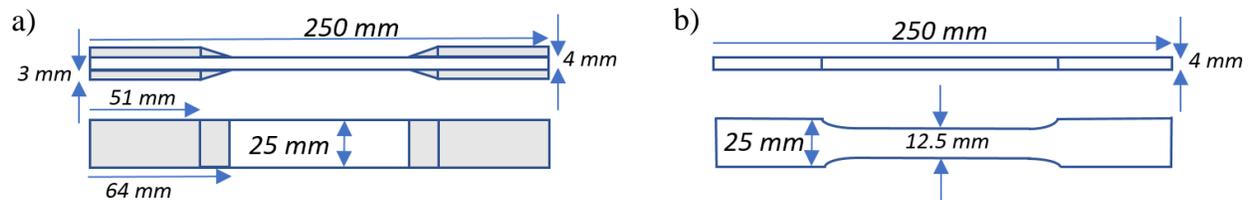


Figure 3: Test specimen geometry: a) Tabbed flax/epoxy composite with tabs; b) Pure matrix having dog-bone shape

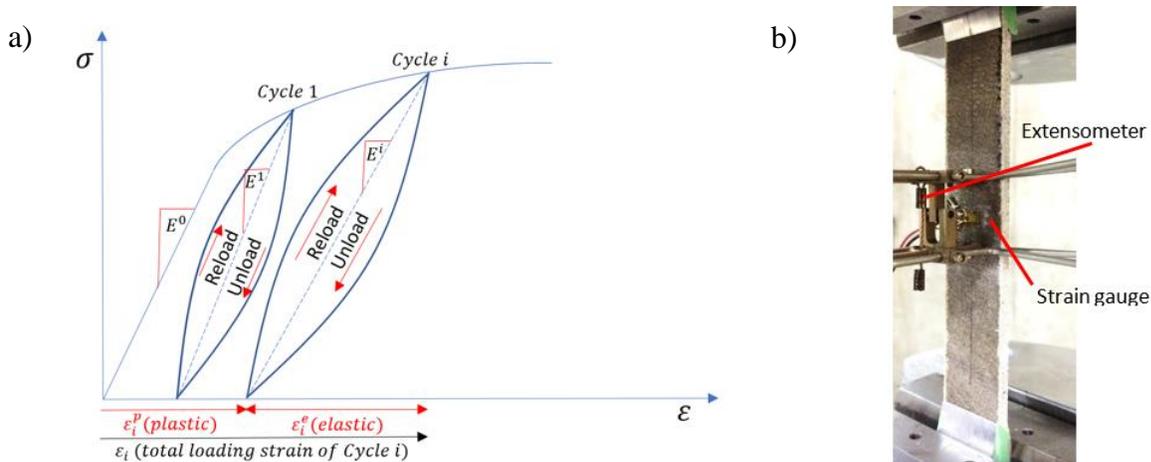


Figure 4: a) Testing procedure illustration; b) Test setup [11]

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3.3 Mesoscale Damage Theory (MDT)

Part of *Continuum Damage Mechanics* (CDM), MDT predicts damage and permanent strain development in elementary plies of fibrous composites. Damage is assumed to uniformly appear and progress through the orthotropic elastic-plastic material, as well as vary from ply to ply. It is defined as the total area of defects S_D normal to \vec{n} . A full description of the model with examples can be found in references [20 - 22].

$$D = \frac{S_D}{S} \quad (1)$$

3.3.1 Modified Mesoscale Damage Model (MMDM)

3.3.1.1 Single Ply

Developed within an irreversible thermodynamic framework, our MMDM uses the Gibbs Free Energy function as the thermodynamic potential of a single ply:

$$\mathcal{G} = -\frac{1}{2} \boldsymbol{\sigma} : \tilde{\mathcal{L}}^{-1} : \boldsymbol{\sigma} - \boldsymbol{\alpha} : \boldsymbol{\sigma} (T - T_0) + c_0 \left([T - T_0] - T \ln \left(\frac{T}{T_0} \right) \right) - s_0 T + H(\mathbf{p}) \quad (2)$$

where bold letters represent sets of numbers, and the following are:

$:$ – colon product

\mathcal{L} & $\tilde{\mathcal{L}}$ – stiffness tensor & damaged material stiffness tensor respectfully

$\boldsymbol{\alpha}$ – Thermal expansion tensor

T_0 – Reference temperature

c_0 – reference specific latent heat

s_0 – reference specific entropy

\mathbf{p} – a set of internal variables related to plasticity mechanisms

$H(\mathbf{p})$ – a set of plastic hardening related functions

Taking the partial derivative of $H(\mathbf{p})$ as $\mathbf{h}(\mathbf{p}) = \frac{\delta H}{\delta \mathbf{p}}$, allows one to express strain ($\boldsymbol{\varepsilon}$) and local entropy production (γ_{loc}) as [1]:

$$\boldsymbol{\sigma} = \tilde{\mathcal{L}}(\boldsymbol{\varepsilon} - \boldsymbol{\alpha}(T - T_0) - \boldsymbol{\varepsilon}^p) \quad \& \quad \gamma_{loc} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_p - \mathbf{h}(\mathbf{p}) : \dot{\mathbf{p}} \quad (3)$$

where $\dot{\boldsymbol{\varepsilon}}_p$ is the time derivative of the plastic strain tensor. The internal variable set \mathbf{p} represents plastic yield surfaces, and each variable of the set is defined as a function of the stress in the damaged material [1]:

$$\boldsymbol{\sigma} = \tilde{\mathcal{L}} : \boldsymbol{\varepsilon} \quad (4)$$

Considering the same strain state, the effective stress of the material can be expressed in terms of the stiffness tensor and strain. Since the effective stress is a representation of actual stress, it can be expressed in terms of the average stress [1]:

$$\tilde{\boldsymbol{\sigma}} = \mathcal{L} : \boldsymbol{\varepsilon} = \mathcal{L} \tilde{\mathcal{L}}^{-1} : \boldsymbol{\sigma} \quad (5)$$

The heart of this model lies in the expression of mean elastic strain energy density (E_D), in terms of effective stresses. It is important to note that the MMDM was developed for a 3D element; therefore, the energy density function contains several added terms compared to the original formulation. Moreover, theories based on the works of Ladeveze et al [21] often use the square bracket notation $\langle \ \rangle_+$, meaning that only under tensile loads damage and plasticity develops. However, from experimental data, it was evident that this is not the case for Flax. Therefore, the square bracket notation was removed and the mean elastic strain energy density function appears as follows:

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$$\begin{aligned}
 2E_D &= \boldsymbol{\sigma} : \tilde{\mathcal{L}}^{-1} : \boldsymbol{\sigma} \\
 &= \frac{\sigma_{11}^2}{E_1^0(1-D_1)} - 2 \frac{\nu_{12}}{E_1} \sigma_{11} \sigma_{22} - 2 \frac{\nu_{13}}{E_1} \sigma_{11} \sigma_{33} \\
 &\quad + \frac{\sigma_{22}^2}{E_2^0(1-D_2)} - 2 \frac{\nu_{32}}{E_3} \sigma_{22} \sigma_{33} \\
 &\quad + \frac{\sigma_{33}^2}{E_3} + \frac{\sigma_{12}^2}{G_{12}^0(1-D_{12})} + \frac{\sigma_{13}^2}{G_{13}} + \frac{\sigma_{23}^2}{G_{23}}
 \end{aligned} \tag{6}$$

, where 11, 22, 12 represent the fiber, transverse, and shear directions respectfully.

Thermodynamic Forces (or damage energy release rates) associated with the damage variables, are defined by Lemaitre and Chaboche [19] in terms of density, thermodynamic potential, and damage. These forces govern damage propagation in a way where some previous maximum value must be exceeded for additional damage to occur [20]:

$$Y_{11} = \frac{\sigma_{11}^2}{2E_1^0}; \quad Y_{22} = \frac{\sigma_{22}^2}{2E_2^0}; \quad Y_{12} = \frac{\sigma_{12}^2}{2G_{12}^0} \tag{7}$$

Damage mechanisms in fiber and shear-transverse directions were decoupled as in the works of Ladeveze and Le Dantec [25]:

$$Y_f = \sqrt{Y_{11}} \quad | \text{Fiber damage and fracture in fiber direction} \tag{8}$$

$$Y_{ts} = \sqrt{Y_{12} + b_{ts} Y_{22}} \quad | \text{Matrix cracking \& fiber - matrix debonding} \tag{9}$$

, where b_{ts} is a coupling constant.

Shear and transverse damage evolution appears as originally formulated in MDT [20], with a linear function describing the fiber damage evolution under compressive loads [1]:

$$\Phi_{D_{11}} = \frac{Y_f - Y_f^0}{Y_f^c} - D_{11} \leq 0, \quad \dot{D}_{11} \geq 0, \quad \Phi_{D_{11}} \dot{D}_{11} = 0 \tag{10}$$

$$\Phi_{D_{22}} = \frac{Y_{ts} - Y_t^0}{Y_t^c} - D_{22} \leq 0, \quad \dot{D}_{22} \geq 0, \quad \Phi_{D_{22}} \dot{D}_{22} = 0 \tag{11}$$

$$\Phi_{D_{12}} = \frac{Y_{ts} - Y_s^0}{Y_s^c} - D_{12} \leq 0, \quad \dot{D}_{12} \geq 0, \quad \Phi_{D_{12}} \dot{D}_{12} = 0 \tag{12}$$

where $\Phi_{D_{ij}}$ is the damage function of the corresponding damage D_{ij} ; while $Y_f^0, Y_f^c, Y_t^0, Y_t^c, Y_s^0,$ and Y_s^c are material-specific parameters to be determined [1].

Inelastic Flax-epoxy response is formulated as in the standard MDT, where the total strain is decomposed into elastic and inelastic strains. A set of elastic domain functions are formulated using effective stresses, and identically to the standard MDT formulation, they are assumed to evolve according to an isotropic power law [1]:

$$\Phi_f^p = \tilde{\sigma}_f^{eq} - h_f(\tilde{\varepsilon}_f^p) - \sigma_f^0 \leq 0, \quad \dot{p}_f \geq 0, \quad \Phi_f^p \dot{p}_f = 0 \tag{13}$$

$$\Phi_{ts}^p = \tilde{\sigma}_{ts}^{eq} - h_{ts}(\tilde{p}_{ts}) - \sigma_{ts}^0 \leq 0, \quad \dot{p}_{ts} \geq 0, \quad \Phi_{ts}^p \dot{p}_{ts} = 0 \tag{14}$$

where

$\tilde{\sigma}_f^{eq}$ & $\tilde{\sigma}_{ts}^{eq}$ – effective stress components which influence the evolution of plasticity

Φ_f^p – inelastic behavior function in the fiber direction

Φ_{ts}^p – inelastic behaviour function in the transverse-shear direction

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$h_f(\tilde{\varepsilon}_f^p) = \beta_f (\tilde{\varepsilon}_f^p)^{\alpha_f}$ – power law shaped hardening function dependent on the fiber-direction cumulative effective inelastic strain ($\tilde{\varepsilon}_f^p$)

$h_{ts}(\tilde{p}_{ts}) = \beta_{ts} (\tilde{\varepsilon}_{ts}^p)^{\alpha_{ts}}$ – power law shaped hardening function dependent on the transverse-shear direction equivalent cumulative effective inelastic strain (\tilde{p}_{ts})

3.3.1.2 Multi-ply Model

Once the behavior of each individual ply is calculated, a homogenization procedure is required to determine the overall composite behavior. Periodic homogenization, based on the works of Bensoussan et al. [23] and Sanchez-Palencia [24], was chosen as the working procedure. This iterative approach allows the use of 3D loadings and has been successfully implemented with non-linearly behaving materials such as shape-memory alloys [25].

3.4 Implementation

The model was implemented using SMART+ libraries (<http://www.lem3.fr/chemisky/smartplus>). Damage condition related to $\Phi_{D_{ij}}$ and plasticity conditions related to Φ_i^p , compose the five non-linear equations numerically treated as described in [25], and used for multi-scale modeling. The following is a summary of the numerical procedures performed during simulations. An in-depth explanation can be found in [25].

3.5 Parameter identification

Material constants have been taken from the works of Mahboob et al. [28]; which compare well with previously published values by other authors. Parameters related to damage and plasticity have been identified using two open-source global optimization algorithms from scipy.optimize libraries [27]. *Basin-Hopping* was used for coarse optimization, and *Differential-Evolution* was used to refine the result. Since the model output and the experimental result for each specimen contained the same amount of discrete points, the following formula was used as a simple cost function (C.F.), minimizing the difference between the experimental and predicted strains:

$$C.F. = \sum_{i=1}^{i=m} \left[a * \left(\sum_{i=1}^{i=n} |\varepsilon_{11}^{exp} - \varepsilon_{11}^{model}| \right) + (1 - a) * \left(\sum_{i=1}^{i=n} |\varepsilon_{22}^{exp} - \varepsilon_{22}^{model}| \right) \right] \quad (15)$$

,where m is the number of specimens of different orientations, n is the number of discrete stress increments per specimen, and a is a weight factor, giving priority to a better fit in the longitudinal direction.

4 VALIDATION, RESULTS, AND DISCUSSION

The MMDM developed by Mahboob et al. [1] applied to a tensile case was validated in for Carbon/Epoxy (T300/914) as well as Flax/Epoxy laminates. Similarly, validation in compression was executed for E-glass/Polyester and Flax/Epoxy laminates.

4.1 E-glass in Polyester and Epoxy

Figure 6a presents a comparison of simulated stress-strain response for E-glass/Polyester laminates in compression with various fiber orientation versus experimental data published by Amijima and Adachi [31]. It was observed that a slight divergence occurs in the $\pm 30^\circ$ specimen at high strain values; nonetheless, the MMDM remains an overall robust and reliable tool for damage response predictions. Figure 6b shows superimposed graphs of experimental and simulated stress-strain response of E-

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glass/Epoxy specimens under tension. Here, it was assumed that damage and plasticity in both tension and compression cases evolve according to the previous established formulations seen in Section 3.3.1.

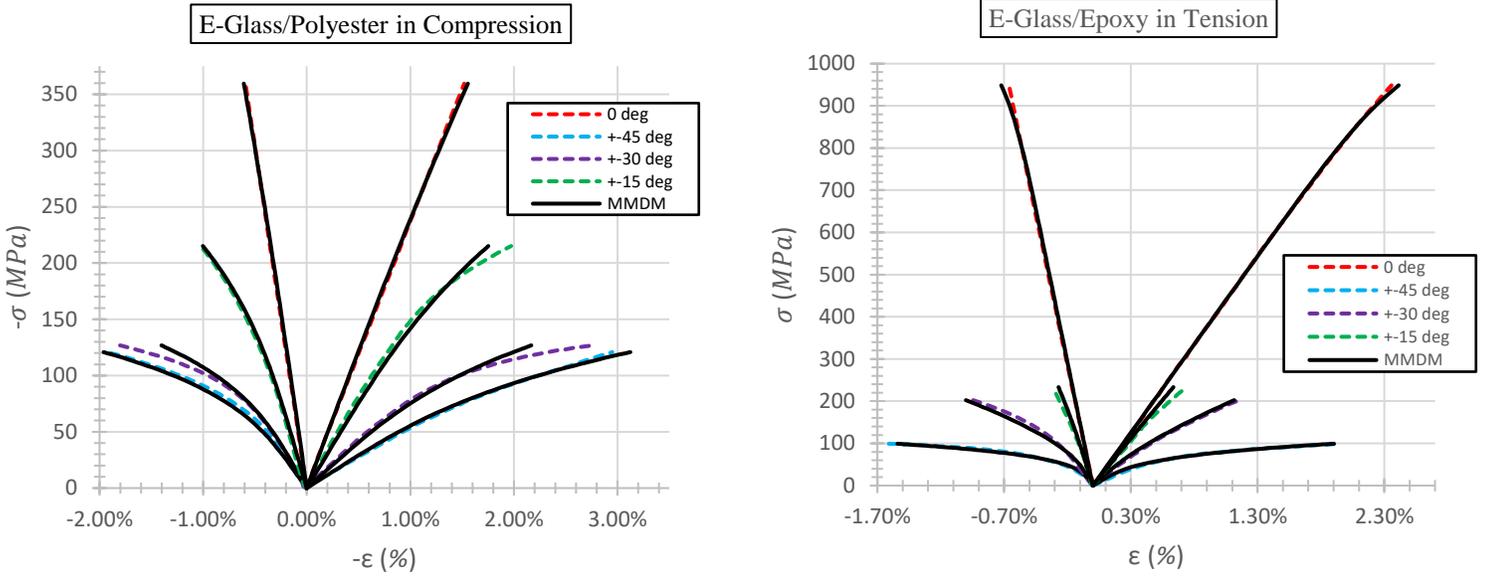


Figure 5: a) E-glass/Polyester compressive mechanical response, b) E-glass/Epoxy tensile mechanical response

4.2 Flax/Epoxy

Standart MDT publications perform cycled load-unload tests on $[0]$, $[90]$, $[\pm 45]_S$, and $[\pm 67.5]_S$ laminates, in order to determine material parameters [20, 21]. In this study, the same ply orientations were used to identify Flax/Epoxy compressive parameters via the optimization methods discussed above. At least four monotonic and/or multiple-cycled progressive loading tests were performed on each laminate and used in parameter identification; thus, the identified parameters are listed in Table 2. The simulated results can be seen in Figure 6; noting that in order to maintain clarity, only one cycled test is shown per laminate. It is clearly noticeable that for $[0]$ and $[\pm 67.5]$ orientations model the material behaviour perfectly even at high strain rates. The $[\pm 45]$ plot matches perfectly on the longitudinal side, however, the transverse direction does not match as well as the other orientations, which could be due to unaccounted buckling effects or interlaminar ply re-orientation. In Mahboobs’s tensile study [1], the $[\pm 45]$ orientation was the most problematic as well. Lastly, for the transverse orientation, i.e. $[90]$, it was found that while its damage evolution follows a similar curve as for $[\pm 45]$ and $[\pm 67.5]$, its plasticity evolution curve is of an exponential shape, and not a power with a fractional exponent as in the $[\pm 45]$ and $[\pm 67.5]$ cases. This means that the model can predict the overall material behaviour and can be applied to only monotonic loading cases for laminates with fibers running in the transverse direction.

Material Property	E_{11}^0 (MPa)	ν_{12}^0	E_{22}^0 (MPa)	ν_{21}^0	G_{12}^0 (MPa)
	31928	0.087	5237	0.396	1660
Fiber Direction	Y_f^0 ($\sqrt{\text{MPa}}$)	Y_f^c	σ_f^0 (MPa)	α_f	β_f
	0.01	1.64	5.653	0.445	2998
Shear Damage	Y_{12}^{max} (MPa)	Y_s^0 ($\sqrt{\text{MPa}}$)	Y_s^c ($\sqrt{\text{MPa}}$)		
	1.263	0.001	2.32		

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Transverse coupled damage	b	Y_{22}^{max} (MPa)	Y_t^0 ($\sqrt{\text{MPa}}$)	Y_t^C ($\sqrt{\text{MPa}}$)
	0.8	5.03	0.0128	2.65
Transverse-Shear yield & inelasticity	A_{ts} (MPa)	σ_{ts}^0	α_{ts}	β_{ts}
	0.79	10.503	0.45	1170

Table 2: Identified model parameters for Flax/Epoxy laminate subjected to compressive loads

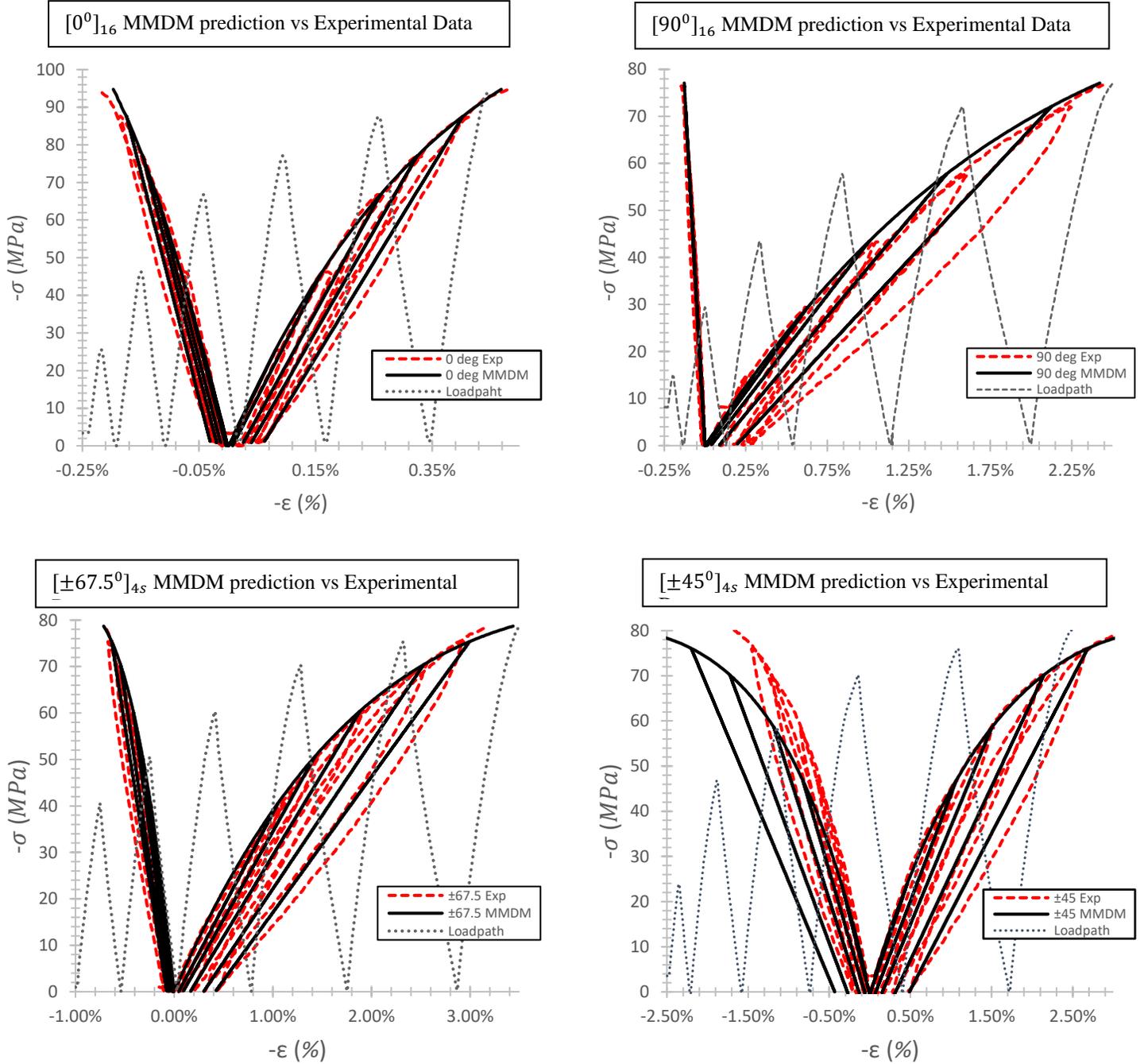


Figure 6: Flax/Epoxy compressive mechanical behavior for composites with fibers of various orientations

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4.3 Further Discussion and Future Work

As seen in Figure 6, it is obvious that flax-reinforced laminates experience damage and plasticity under compressive loads. Overall, the proposed MMDM is successfully predicting the mechanical behaviour of NFCs. There are three major future works goals planned, which will improve the model's predicting capabilities. Firstly, it was observed that plasticity evolution in all specimen orientation is of a power curve with a fractional exponent shape except for transverse, which resembles an exponential curve. Since the model is formulated such that shear and transverse effects are coupled with a linear coupling parameter, it is unable to convert the power-curve shaped behaviour into an exponential one. Therefore, future work includes exploring more complex types of coupling parameters which will enable the transverse direction plasticity to evolve as it was observed in experimental data. The second major goal is to improve the prediction of the $[\pm 45]$ transverse behaviour, by introducing a buckling model in the constitutive equations. Lastly, this model will be implemented in mainstream design software such as ABAQUS, which will elevate the model's predictive capabilities from a single 3D element to complex multi-element shapes.

5 CONCLUSION

Natural fiber-reinforced composites present an untapped source of environmentally friendly, sustainable, and cost effective substitute to composite reinforced with synthetic fibers. The impeding factor of NFC's widespread use as load-bearing components, is the lack of robust and accurate predictive tools that can capture their non-linear mechanical behavior.

A Modified Mesoscale Damage Model was recently developed by the current authors [1], and has been demonstrated to accurately predict Flax-reinforced composite mechanical behavior in tension. This study modified the damage evolution law in the fiber direction, and demonstrated the model's ability to predict NFC's material behavior under compressive loads. Also, this model is very versatile, and can be easily adapted to predict the mechanical behavior of various types of composite materials as shown in the validation section.

Incorporating buckling into this model and implementing into a modern finite element software will allow engineers to use NFCs for load-bearing applications with confidence, which will promote the use of eco-friendly materials in various engineering applications.

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