Computational Modeling of Natural Fiber Composites: Assessing the Accuracy of Coupled Simulation for Predicting Mechanical Properties

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Abstract -The increasing use of natural fiber composites (NFCs) as a substitute for synthetic fibers like glass and carbon fibers is driven by the need to reduce greenhouse gas emissions and promote environmental responsibility within engineering industries. A key challenge is to fully understand the connection between fiber orientation and the mechanical behavior of wood fibers (WFs) in these composites. This study evaluates a computational method coupling injection molding simulation with finite element analysis, using fiber orientation tensor mapping to analyze wood fiber composites (WFCs). The approach involves tensile testing of specimens with varying fiber orientations (0°, 45°, and 90°) and comparing the results with numerical simulations. Key findings highlight the anisotropic nature of WFCs, with 0° oriented specimens showing distinct mechanical behavior compared to 45° and 90° specimens. The study also demonstrates the effectiveness of the computational models, with strong agreement between experimental and simulation results. This research enhances the understanding of WFC mechanics, crucial for optimizing structural integrity, cost-efficiency, and sustainability in real-world applications, and suggests that WFs exhibit less breakage than glass fibers, indicating their potential durability.

Keywords: Fiber reinforced composites, mechanical properties, finite element modeling, material simulation, stress-strain behavior, composite mechanics.

Introduction

This research focuses on the computational modeling and mechanical analysis of natural fiber composites (NFCs), which are gaining importance due to their eco-friendly properties and potential to replace synthetic fibers in industries like automotive. The study is motivated by growing environmental concerns and European Union regulations mandating vehicle recyclability. NFCs offer benefits such as reduced weight and cost, but their mechanical behavior is highly dependent on fiber orientation and distribution, making accurate prediction challenging. This thesis investigates computational tools—primarily finite element analysis (FEA)—to evaluate the influence of fiber alignment on mechanical performance. Injection molding simulation using Autodesk Moldflow is employed to predict fiber orientation tensors, which are then transferred to finite element models through Digimat-MAP. This mapping is essential for coupling molding simulations with structural analysis. The study integrates physical testing data to enhance model accuracy and uses LS-DYNA software to simulate mechanical responses under different conditions. By combining experimental and numerical methods, the research aims to improve the reliability of NFC performance predictions. The ultimate goal is to develop an efficient modeling workflow to support sustainable design practices, particularly in automotive applications such as those pursued at Volvo Car Corporation (VCC), while acknowledging the need for continued refinement.

Literature Review –

Fiber-Reinforced Composites (FRCs) are increasingly employed in engineering applications due to their high strength-to-weight ratio, durability, and tailored mechanical properties. Accurate prediction of their behavior under various loading conditions is essential for optimizing structural designs. This literature review synthesizes recent research that explores advanced modeling and simulation techniques aimed at enhancing the predictability and performance analysis of FRCs.

Zhang, Liu, and Zhang [1] propose a multiscale computational framework combining micromechanical modeling and finite element analysis (FEA) to bridge microscale fiber-matrix interactions and macroscale mechanical responses. By incorporating progressive damage modeling and homogenization techniques, their approach accurately simulates failure mechanisms such as matrix cracking and fiber breakage. The study emphasizes the growing use of machine learning and multiscale methods in computational mechanics to improve both accuracy and efficiency.Islam, Alam, and Mansur [2] delve into interfacial debonding in FRCs using FEA integrated with cohesive zone modeling (CZM). Their work demonstrates how interfacial failures influence load transfer and overall composite strength, offering better insight than traditional analytical methods. Their findings align with current trends in damage mechanics, highlighting the critical role of interfacial modeling in composite analysis.Wang, Li, and Zhang [3] investigate damage evolution under cyclic loading using micromechanical models and computational homogenization. Their FEA-based approach effectively captures matrix cracking, fiber failure, and interfacial debonding. By applying strain energy-based damage evolution laws, they underscore the influence of fiber orientation and matrix toughness on fatigue behavior, further reinforcing the importance of microstructural details in composite modeling.Singh and Gupta [4] focus on progressive damage simulation in fiber-reinforced polymer composites using CDM and CZM. Their research, supported by material degradation laws, simulates multiple failure modes under different loading conditions. This work aligns with the evolution of high-fidelity simulations and suggests a growing role for machine learning and phase-field methods in modeling composite damage.

Kumar, Singh, and Sharma [5] address the impact behavior of FRCs, utilizing advanced FEM techniques, including XFEM and CZM. They highlight how interfacial bonding and dynamic loading affect energy absorption and delamination. Their research supports the integration of dynamic solvers and multiscale methods in enhancing impact resistance and structural reliability.Chen, Li, and Yang [6] introduce machine learning algorithms such as ANNs and SVMs to predict mechanical properties of FRCs. This data-driven approach presents a cost-effective alternative to experimental testing, facilitating rapid material design and optimization based on key input variables like fiber content and matrix characteristics.Zhang, Xu, and Zhao [7] use multiscale RVE-based modeling to estimate elastic and thermal properties of FRCs. Their approach provides insights into how microscale structures influence global behavior under mechanical and thermal loads.Hossain, Kabir, and Islam [8] develop an anisotropic phase-field model for simulating intra-laminar fracture in composites. Their Abaqus-based model successfully predicts crack initiation and propagation, validated through experimental comparisons.Nguyen et al. [9] explore the effects of imperfect fiber-matrix interfaces via computational homogenization, revealing their significant influence on stiffness and strength.Lastly, Patil, Kulkarni, and Joshi [10] investigate delamination under impact using CZM, identifying key parameters like impact energy and loading rate that affect damage progression.Collectively, these studies reflect a clear trend toward integrated, multiscale, and high-fidelity modeling techniques to improve the predictive capabilities and reliability of fiber-reinforced composites in engineering applications.

Methodology

The methodology employed in this study is illustrated in following Figure, and it involves several key steps.

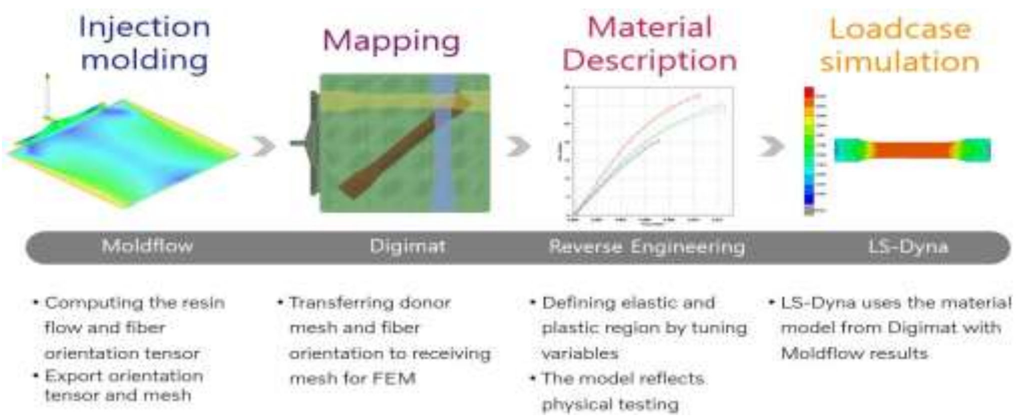

Figure1.1. Theworkflowemployedforanalyses

Figure 1.2 Specimens cut out from three plaques at three different angles; 0, 45, and 90 degrees from left to right.

First, injection molding simulation is conducted using Autodesk Moldflow Insight Basic to calculate resin flow and determine the fiber orientation tensor within the composite material. The orientation tensor and corresponding mesh data are then extracted from the Moldflow simulation. Digimat-MAP is used to map the orientation data, transferring fiber orientation details and mesh information from the donor mesh data to the receiving mesh, which is essential for integrating Moldflow data with finite element models (FEMs) for further analysis. The material behavior, including elastic and plastic regions, is defined within the material model, with fine-tuning of variables to accurately represent the composite's mechanical response, incorporating physical testing data to enhance the accuracy of simulations. Finally, LS-DYNA software is used for FEM simulation to analyze the material's behavior, strength, and performance under various conditions.

After the work in Digimat-MF is finished, the optimized values of the fiber orientation are obtained through a reverse engineering process. It involves comparing measured and simulated stress-strain [34] as showninFigure4.11.Thisisachievedbyidentifyingvariables, such as elastic modulus, Poisson's ratio, yield strength, and linear hardening. This ensures thatthematerialmodelreflectsthereal-worldbehaviorofthecompositematerial, leading to more reliable predictions of mechanical properties and performance. Theleftgraphshowsthedifferencesbetweenmodelpredictionand tensile test before the process, the right graph shows optimized values after the process.The polymeric material used in this study is Stora Enso Dura Sense PP-NF40, which consists of a polypropylene (PP) matrix reinforced with 30 weight-% coniferous wood and 10 weight-% engineered WF, with fiber dimensions of 1.5mm length and 0.5mm width. The material's properties, including density, mold temperature, melt temperature, elastic modulus, Poisson's ratio, and shear modulus, are provided by Stora Enso. Uniaxial tensile testing is conducted at the Material Laboratory Center in VCC to evaluate the mechanical properties of DuraSense PP-NF40 under tension and to provide data for material characterization and comparison with simulation results, including fiber orientation and distribution effects. The testing results are also used for validation and calibration of computational models and simulations to predict the mechanical behavior of natural fiber-reinforced plastic. Specimens are prepared from injection-molded plaques with dimensions of 140mm×140mm×2mm, following the recommended processing protocol from Stora Enso. Dogbane-shaped specimens are cut from three plaques oriented at 0 degrees, 45 degrees, and 90 degrees using water jet cutting, and then dried in an oven to remove moisture. The location of each specimen on the plaque is recorded to investigate the effect of fiber orientation and distribution on mechanical properties. Specimens oriented at 0°, 45°, and 90° are selected for comparison with strength analysis in relation to fiber orientations.

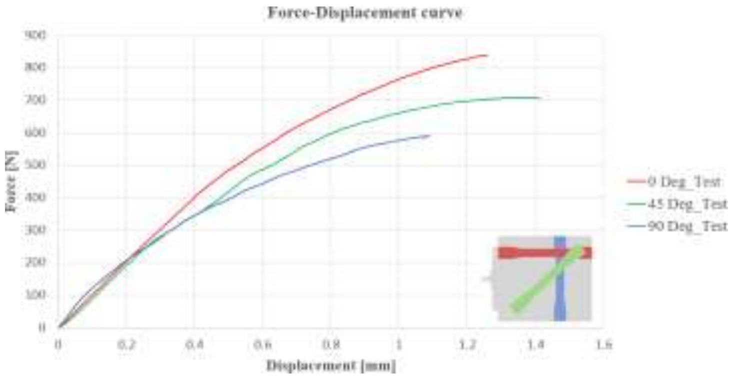

Figure1.4 Experimental Force-displacementcurveforS5from0degrees,S2from45 degrees, and S4 from 90 degrees.

Data sheet values of material properties for Dura Sense PP-NF40 provided by Stora Enso are presented in table 1.1

Table1.1 DensityandmechanicalpropertiesdataofDuraSensePP-NF40 [26]

Density	1111	kg/cm³
Mold Temp	60-90	℃
Melt Temp	180-210	℃
Elastic Modulus [E1]	3856	MPa
Elastic modulus [E2]	2619	MPa
Poisson's ratio[v12]	0.45	-
Poisson's ratio [v23]	0.71	-
Shear modulus[G12]	1081	MPa

The study utilized the Aramis testing machine to apply axial loads while capturing real-time displacement and strain data for generating stress-strain curves. Wood fiber (WF) characteristics in composites were examined using optical microscopy, revealing aspect ratios of approximately 3.0–3.2, which significantly influence mechanical properties like tensile strength and stiffness. Chemically treated specimens improved fiber visibility. Fiber volume fractions were assessed through both a mathematical model and MATLAB image analysis, yielding consistent results around 36%. MATLAB also quantified fiber orientation, aligning well with Moldflow simulation data, thereby validating the accuracy of combined optical and computational techniques in characterizing composite microstructure.

Table 1.2 The volume fraction by mathematical calculation and MATLAB calculation with capture image on microscope.

	Matrix (%)	Wood fiber (%)
Mathematical	64.1	35.9
MATLAB with image	63.5	36.4

Analysis-

This study uses injection molding simulation with DuraSense PP-NF40 to analyze fiber orientation in a rectangular plaque. Results show strong fiber alignment in the flow direction (Txx), especially at the edges, and random orientation perpendicularly (Tyy). Comparative analysis with PP-GF30 indicates higher alignment in Txx.

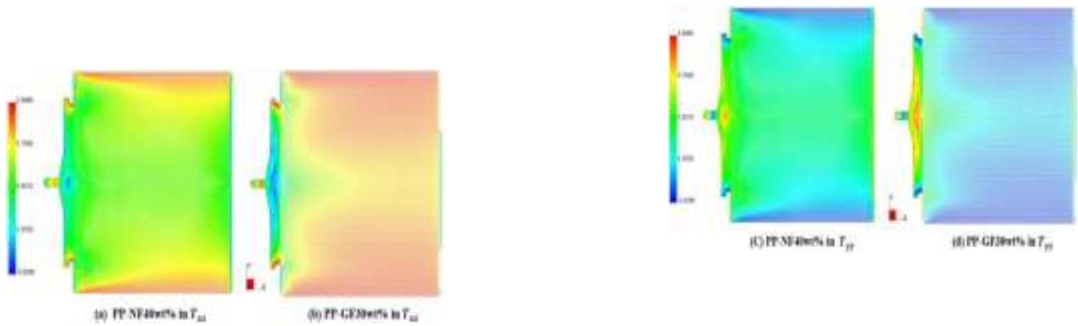

Figure 1.5 Fiber orientations of PP-NF40wt% and PP-GF30wt% in Mold flow analysis. (a) PP-NF40wt%inT_{xx}, (b)PP-GF30wt%inT_{xx}, (c)PP-NF40wt%inT_{yy},(d)PP-GF30wt%inT_{yy}.

FEM Analysis

A FEM analysis using Mold flow fiber orientation and a Digimat failure model was validated against tensile tests for specimens at 0°, 45°, and 90°. While predictions matched well at 0°, minor deviations occurred at 45° and significant discrepancies at 90°, revealing limitations in accurately modeling off-axis mechanical behavior.

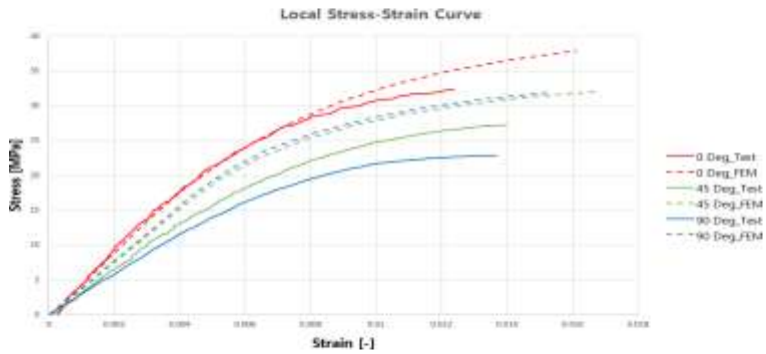

Figure1.8 Stress-Straincurvecomparisonbetween FEMsimulationandtensiletesting.

Results and Discussion

The developed computational workflow effectively integrated multi-domain simulation tools, ensuring efficient data exchange and emphasizing the need for robust data architecture in multi-scale modeling. Injection molding simulations accurately predicted fiber orientation, though limitations in Digimat's material data and parameters introduced uncertainties. The mesh-mapping algorithm performed well, despite minor interpolation errors near complex geometries. Morphological analysis revealed that wood fibers (WFs) have non-uniform diameters, elliptical shapes, lower fragmentation than glass fibers (GFs), and greater anisotropy. Future work should focus on refining material characterization, improving fiber orientation models, benchmarking simulation workflows, enhancing interoperability, and exploring the sustainability and performance of natural fiber composites (NFCs).

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