

THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING IN SOLID AND
STRUCTURAL MECHANICS

Modelling and simulation of the compressive behaviour of fibre-reinforced polymers

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To my family

Abstract

Fibre-reinforced polymers (FRPs) are lightweight materials with high specific strength and stiffness. These materials are increasingly substituting metallic alloys in automotive, aerospace, and civil engineering structures. In applications such as aircraft fuselage panels, automotive monocoques, wind turbine blades, hydrogen pressure vessels, they are often exposed to significant compressive loads. However, their compressive strength is typically lower than their tensile strength in the primary load-bearing direction, making accurate predictions of compressive failure essential for safe and efficient structural design.

FRPs are inherently hierarchical materials, with reinforcing fibres 5-25 μm in diameter in most cases, orders of magnitude smaller than the structural scale. Unlike most metals, FRPs are highly anisotropic and feature many load-dependent complex failure modes. Recent advances in experimental and imaging techniques have made it possible to examine the failure processes post mortem and in real-time, contributing to understanding the material behaviour and giving rise to new, physically based material models.

This thesis presents a modelling framework that connects different compressive/shear failure modes based on the underlying micromechanics. Using the physical connection between these separate failure modes simplifies material parameter calibration. Adoption of a simplified micromechanical representation makes it possible to efficiently account for spatial variation in morphological features, such as fibre misalignment and inhomogeneous fibre volume fraction.

The model is calibrated for a carbon-fibre reinforced polymer using simple load cases from the Third World-Wide Failure Exercise, followed by the generation of biaxial failure envelopes. The predictions are compared with phenomenological and physically based stress-based failure criteria. Additionally, a compression test campaign on a different carbon-fibre reinforced polymer material is also considered, featuring a number of unidirectional and multidirectional laminates. After parameter calibration on the unidirectional laminates, the model predicted the compressive strength of six multidirectional laminates with an average deviation of 6.14% from the experimental means.

Keywords: Fibre-reinforced polymers, compressive failure, fibre kinking, continuum damage mechanics, homogenisation.

List of Publications

This thesis is based on the following publications:

[A] **Krisztián György Hertelendy**, Renaud Gutkin, Ragnar Larsson, “A micromechanically inspired model for compressive and shear failure in fibre-reinforced composites”. Under review.

[B] **Krisztián György Hertelendy**, Ragnar Larsson, “Comparative study of homogenisation models for the transverse and shear elastic response of UD fibre-reinforced polymers”. Manuscript.

Preface

The work presented in this thesis was carried out from August 2023 to March 2026 at the Division of Computational Mechanics and Materials Engineering, Department of Mechanical Engineering, Chalmers University of Technology (formerly the Division of Material and Computational Mechanics, Department of Industrial and Materials Science). The research received financial support from Horizon Europe through the MSCA Doctoral Network RELIANCE: REaL-time characterisation of ANisotropic Carbon-based tEchnological fibres, films and composites, grant no. 101073040.

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I would also like to thank my friends and colleagues at the division and at Chalmers. The shared lunch breaks, conversations, and laughter made the good days even more enjoyable and helped me through the more challenging ones. I look forward to continuing to explore languages together and sharing our excitement about meatball days at Kåren.

Last but not least, I am deeply grateful to my parents and family, who have always supported me in everything, no matter what.

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Part I

Overview

CHAPTER 1

Introduction

1.1 Background and motivation

The market for fibre-reinforced polymers (FRPs) has grown steadily over the past four decades, as part of a general trend towards weight reduction and lightweight solutions. The global market experienced a compound annual growth rate of 2%-4% in the last ten years and is expected to grow at a rate of 5%-7% until 2030 [1]. The global annual demand for carbon fibres alone has increased from 36.4 kilotonnes in 2008 to 115 kilotonnes in 2023 and is predicted to reach 280.3 kilotonnes in 2030 [2]. The automotive industry dominated the use of FRPs with a global share of 40.2% in 2023 [3], but other sectors such as the aviation, maritime, wind energy, and sports industries also increasingly utilise these materials.

FRPs offer numerous advantages, making them highly attractive for a range of engineering applications. Their high mass specific mechanical properties make them an appealing choice for sectors where weight reduction is critical and structural requirements are moderate to high. Typical structural steels have a tensile modulus of around 207 GPa and a density of 7.8 g/cm³ [4]. Aluminium, a traditional lightweight material, has roughly one third of the

density and stiffness of steel, around 69 GPa, and 2.7 g/cm^3 [4], resulting in mass-specific stiffness close to that of steel. As an example, IM7/8552 prepregs with 57.7% fibre volume fraction possess a tensile modulus of 67 GPa in the fibre direction at a density of 1.57 g/cm^3 [5], a 60% increase in mass-specific stiffness compared to structural steel. The difference in mass-specific strength properties is even more notable; the IM7/8552 composite mentioned above has a tensile strength of 2724 MPa in the fibre direction [5], which exceeds the ultimate tensile strength of most structural steel materials even in absolute terms, although having a fraction of the density of steel. Another advantage is their excellent corrosion resistance that makes them ideal for use in corrosive environments, such as the wind energy and maritime sectors.

Unidirectional FRPs often have an order of magnitude higher stiffness and strength in the direction of the reinforcing fibres compared to the transverse direction. By stacking composite plies with different orientations, a wide range of laminate properties can be achieved, offering a flexible design framework where the mechanical behaviour can be tailor-made for specific applications.

FRPs are often used in safety-critical areas, such as primary structures in aircraft, wind turbine blades, hydrogen pressure vessels, monocoques, and crash structures. As a few examples, the Boeing 787 Dreamliner and the Airbus A350 XWB aircraft models are constructed with over 80% composite materials by volume fraction [6], and the blades of modern wind turbines are also predominantly made of composite elements [7]. In turn, strict safety requirements led to extensive research on their constitutive behaviour and failure mechanisms, which have been an active area of research since their appearance. In many applications, including the examples above, composite panels may be loaded in compression. As the longitudinal compressive strength is generally lower than the tensile strength, it often becomes a design parameter of composite structures. However, predicting the failure of composites in compression is a particularly complex problem, as the failure mode is closely related to the microstructure of the material, sensitive to manufacturing-induced imperfections, and generally requires more extensive modelling considerations [8].

Modelling and understanding the micromechanics behind the different failure modes have evolved significantly. The earliest failure models were primarily phenomenological stress/strain-based criteria derived from empirical observations. The maximum strain and maximum stress criteria [9] apply a

component-wise limit on the strain or stress tensor, where the limits are usually derived from uniaxial and shear tests. Quadratic criteria, such as the theories of Tsai-Hill [10] and Tsai-Wu [11] consider the interaction between different stress components qualitatively. A step towards physically based models was the Hashin criterion [12], [13] that differentiates between different failure modes, such as fibre tension, fibre compression, matrix tension, and matrix compression, but the expressions were still mainly empirical. Later models considered the micromechanics behind the failure process more explicitly, and are therefore generally classified as physically based criteria. These include the Puck criterion [14] and the LaRC05 model [15] developed at the Langley Research Center.

A common feature of the failure theories listed above is that they only predict a failure initiation point based on the stress-state in the material, until which the composite is often assumed to follow a linear elastic constitutive law. FRPs are quasi-brittle materials with generally low strain-to-failure values, but depending on the lay-up and load case, significant nonlinearities and complex behaviour can be observed both before and after failure initiation. With the development of computational techniques and the increase in computing capacity, research has progressed towards models more explicitly resolving the underlying micromechanics and surrogate models calibrated using micromechanical models [16], [17], [18], [19]. Particularly significant efforts have been made to understand and model fibre kinking failure using micromechanical models, which is the dominant failure mode in longitudinal compression [8], [20], [21], [22].

1.2 Research scope and objectives

This thesis presents the first phase of the development of a computational model for predicting the compressive mechanical behaviour of continuous fibre-reinforced polymers. Investigations are restricted to compression and shear load cases. The material model is formulated for stiff fibres embedded in a softer matrix with moderate to high fibre volume fractions. The experimental data used for validation were measured in carbon and glass fibre-reinforced polymers with thermoset resin materials. The objectives in the first half of the project have been the following:

- Establish a computationally efficient micromechanics-based material

model that considers manufacturing-induced microstructural features, such as the inhomogeneous distribution of fibre cluster orientation and fibre volume fraction.

- Implement the developed model and apply it to compressive strength predictions of unidirectional and multidirectional coupons.
- Assess the compressive strength prediction performance of the model by comparing the predicted results with experimental data and other material routines available in the literature.
- Compare numerically generated biaxial failure envelopes with common stress-based failure criteria.
- Understand the limitations of the model.

2.1 Fibre-reinforced polymers

Fibre-reinforced polymers (FRPs) are a combination of a polymeric matrix material and reinforcing fibres embedded in the matrix. The fibres provide mechanical load-bearing capacity, while the primary functions of the matrix are load transfer between the fibres and environmental protection. They can be classified on the basis of different aspects, e.g. fibre/matrix materials, reinforcement type and shape, or manufacturing method. The most widely used fibre materials are glass, carbon, and aramid, although natural fibres are also becoming more common due to their environmental advantages. Matrix materials are usually divided into two main categories, thermoplastic and thermoset polymers.

The reinforcing fibres may be continuous or discontinuous and can be aligned or randomly oriented. The micromechanics of different reinforcement types can be very different, and therefore models predicting failure are usually only applicable to one family of reinforcement type. In the present thesis, the computational model is established for composites with continuous, aligned fibres. The primary application area is laminated composites but the material routine

can be applied to FRPs of different forms, such as pultruded composites.

Defects are introduced into the composite during the manufacturing process. Air is unavoidably trapped in the resin during its solidification, leading to voids in the final product. A higher void content can negatively impact mechanical performance and therefore in many applications the allowed void content is limited to about 1% [23]. Furthermore, chemical interaction between the resin and the fibres (or the sizing, if present) creates a finite transition zone between the fibre and resin regions known as the interphase region. There are studies investigating the effects of the void content [24], [25], [26], [27] and the properties of the interphase [28], [29], [30], [31], although they are often omitted due to their low content. In the modelling work presented in this thesis, the void and interphase contents are neglected, i.e. the fibre and matrix volume fractions add up to 100%.

2.2 Failure modes in compression and shear

The major failure modes observed in compression and shear, and their possible explanations are summarised in this section.

Under pure longitudinal compression, most FRPs fail in fibre kinking, caused by local imperfections that result in a misalignment between the applied load and the fibre direction. Fibre kinking failure has been extensively investigated experimentally, analytically, and by computational models.

Many recent studies are based on the theoretical works of Budiansky and Fleck [32], [33], which later became known as fibre kinking theory (FKT). They assumed an infinite band of initially misaligned fibres in the composite, and subsequent rotation of the fibres is governed by a balance between the applied compressive stress and the shear resistance counteracting the rotation of the fibres. Due to the strong shear nonlinearity of the composite, its ability to resist further fibre rotation saturates, and the fibres eventually buckle and break locally, leading to the formation of a kink band. Because the entire process occurs very rapidly, capturing the chain of events experimentally became possible only recently by ultra-fast in-situ synchrotron tomography [34] with 50 μs per frame.

For high initial misalignment angles, fibre splitting resulting from high shear stresses in the matrix is observed between misaligned fibres [15]. Fibre splitting might or might not lead to the formation of a kink band, depending on

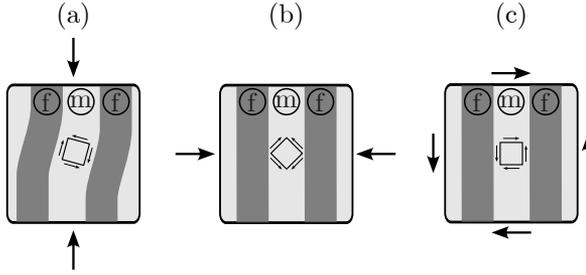


Figure 2.1: Planes of maximum shear in the matrix in (a) longitudinal compression in the presence of initial imperfections, (b) transverse compression, and (c) in-plane shear. \textcircled{f} – fibre, \textcircled{m} – matrix.

the local stress state [15]. However, the two failure modes are described by the same equation in the state-of-the-art LaRC05 failure criterion suggesting that the same root cause leads to failure, namely shearing of the matrix.

The orientation of the fracture plane in pure transverse compression ($53^\circ \pm 2^\circ$ to the loading direction for most technical composites [35]) and the presence of shear cusps on the fracture surfaces in shear tests (see, e.g. [36]) suggest that failure is driven by matrix shear in both load cases. The deviation from the 45° angle expected for pure shear failure was explained in [35] by additional friction forces acting on microcracks, which shift the fracture angle from the plane of maximum shear stress.

Based on the above, it can be concluded that shear localisation in the matrix plays a significant role in the failure of FRPs in every simple compression/shear load case. Fig. 2.1 illustrates the planes of maximum shear in the three cases.

2.3 Modelling considerations

This section summarises the consequences of the observed physical phenomena on the modelling considerations presented in **Paper A**.

The key sources of nonlinearities leading to failure identified in the previous section are material nonlinearity in the form of a nonlinear shear response of the matrix and geometric nonlinearity originating from large rotation of the fibres in the fibre kinking process.

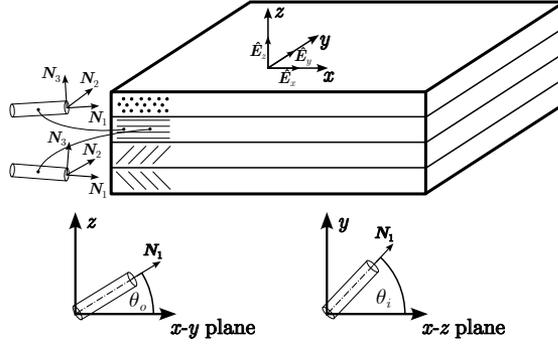


Figure 2.2: Definition of the local and global coordinate systems and in-plane and out-of-plane fibre angles.

The proposed material model is therefore formulated with nonlinear kinematics to properly account for fibre rotation. The constitutive responses of the two constituents are formulated in the form of hyperelastic material models. The stress-strain relations are prescribed in the material configuration using the Green-Lagrange strain tensor \mathbf{E} and the second Piola-Kirchoff stress tensor \mathbf{S} .

The modelling approach presented in **Paper A** is based on a two-phase material model, in which the constitutive response of the composite is derived from that of the constituents via homogenisation. This allows for modelling microstructural inhomogeneities in the sample, such as varying fibre orientation and fibre volume fraction, as shown in Fig. 2.2. Another advantage is direct access to the stress/strain state in the fibre and the matrix, by which the different failure modes can be connected via matrix shear failure.

An important step in the proposed two-phase material model is to obtain the effective composite response in terms of the constituent properties. For composites, this is usually done either with analytical/semi-analytical models that may or may not be micromechanics-based, or by using computational homogenisation on a representative volume element of the microstructure. The first approach is taken in **Paper A**, where a mean-field-based analytical homogenisation scheme is proposed inspired by the underlying micromechanics.

Since the fibres only experience large rotations, but not large stretches, the free energy density function of the fibres is defined such that it corresponds to a transversely isotropic linear elastic law between the second Piola-Kirchoff

stress and the Green-Lagrange strain. The shear degradation of the matrix is a key mechanism in the damage process; therefore, the matrix is modelled using an isotropic constitutive law with continuum damage degrading the deviatoric part of the stress, corresponding to the highlighted material nonlinearity. The real nonlinear shear response is the result of a combined effect of plasticity and material degradation, both represented by continuum damage in the proposed model, narrowing the application area to monotonic loading.

Based on discrepancies in the predicted initial longitudinal shear modulus identified in **Paper A**, the homogenisation problem is revisited in **Paper B**. In this paper, different analytical and computational homogenisation methods are compared in the small strain regime with data from four composite systems with the objective of improving the accuracy of the homogenisation scheme used in the model.

CHAPTER 3

Summary of included papers

This chapter provides a summary of the included papers.

3.1 Paper A

Krisztián György Hertelendy, Renaud Gutkin, Ragnar Larsson

A micromechanically inspired model for compressive and shear failure in fibre-reinforced composites

Under review.

A 3D macroscale continuum damage mechanics model for FRPs is proposed and implemented as a user defined subroutine in Abaqus. The composite response is obtained by a mean-field type homogenisation scheme from the constituents' constitutive laws in a large strain setting. The fibre and matrix are modelled as hyperelastic materials, and the deviatoric part of the stress in the matrix is degraded by continuum damage, mimicking physically observed phenomena in matrix shear-driven failure modes. The model allows for spatially varying fibre volume fractions and fibre orientations. The proposed model was investigated at different levels. At the material point level,

the predicted mechanical response in simple load cases was compared with experimental data and biaxial failure envelopes were generated numerically and compared with physically based stress-based failure initiation criteria. The compressive strength predicting capability for compression coupons was assessed by comparing the simulation responses to experimental data and other well-established material models in the literature.

3.2 Paper B

Krisztián György Hertelendy, Ragnar Larsson

Comparative study of homogenisation models for the transverse and shear elastic response of UD fibre-reinforced polymers

Manuscript.

In this paper, we compare different homogenisation methods for elastic property prediction in FRPs. Analytical, semi-analytical and computational homogenisation methods are investigated. The (semi-)analytical methods include the Halpin-Tsai, Chamis, and bridging models, as well as the homogenisation scheme proposed in **Paper A**. Microstructure representations of various levels of detail are investigated for computational homogenisation, including both random microstructures and idealised unit cells. A Monte Carlo-based simulation is proposed to generate periodic representative volume elements (RVEs) with randomly distributed fibres. Using this method, eight microstructures containing 225 fibres are created. In addition, unit cells representing square and hexagonal packing, and a simplified unit cell with very high computational efficiency are also examined. The comparison is made based on four composite systems, each with a 60% fibre volume fraction.

CHAPTER 4

Concluding Remarks and Future Work

The present thesis presents a modelling framework introduced in **Paper A** to simulate the mechanical response of FRPs in compression-driven load cases. A continuum damage mechanics model with hyperelastic constituents and an effective mean-field homogenisation scheme was proposed and its predictive capabilities evaluated.

The numerical prediction of the initial misalignment angle based on the longitudinal compressive strength showed a close quantitative agreement with the analytical solution of Budiansky using the fibre kinking theory. Biaxial failure envelopes are generated numerically with the calibrated parameters. It was shown that failure prediction of the model follows the LaRC05 criterion in combined longitudinal compression/shear corresponding to fibre kinking / splitting failure, and it is close to the quadratic Hashin criterion in transverse compression/shear corresponding to matrix cracking.

The model was also applied to a compression test campaign in **Paper A**, highlighting its predictive capabilities for different unidirectional and multidirectional laminates. After material calibration on the unidirectional laminates, the model predicted the compressive strength of six multidirectional laminates with an average deviation of 6.14% from the mean experimental

value, lower than two reference material models from the literature.

Paper B dealt with a comparison between different homogenisation schemes to improve the transverse and shear property predictions of the computational model. Unit cells representing square and hexagonal packing, as well as a computationally efficient simplified unit cell featuring 5 finite elements were found to be representative of the transverse and shear elastic properties when the mean value of the angle-dependent properties is taken. It was found that the predictions of the semi-analytical Chamis and bridging models are comparable to those of the random microstructure RVE, although having a fraction of the computational cost. Additionally, the proposed highly efficient simplified unit cell has an accuracy similar to that of random microstructures when the mean value in the transverse plane is taken.

Future work in the project will address the following points:

- The addition of finite-strain plasticity in the computational model to investigate the effects of modelling plasticity on the failure process.
- Digital twins of as-manufactured specimens where morphological features such as fibre direction and fibre volume fraction distribution are mapped on the finite element mesh using X-ray computed tomography.
- Investigation of the importance of modelling inhomogeneities in predicting the longitudinal compressive strength of unidirectional composites.

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