Thermo-mechanical structural modelling of FRP composite sandwich panels exposed to fire

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Thermo-mechanical Structural Modelling of FRP Composite Sandwich Panels Exposed to Fire

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy in Structural Engineering by William T. Ramroth

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2006
The dissertation of William T. Ramroth is approved, and it is acceptable in quality and form for publication on microfilm:

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Chair

University of California, San Diego

2006
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ABSTRACT OF THE DISSERTATION

Thermo-mechanical Structural Modelling of FRP Composite Sandwich Panels Exposed to Fire

by

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Doctor of Philosophy in Structural Engineering
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Professor Petr Krysl, Chair

The goal of this work is to predict the mechanical behavior of FRP composite sandwich structures in naval applications during a fire event. To do this, several models have been developed and integrated. The first is a thermal model—this provides a prediction of temperatures with time resulting from the fire exposure; accounting for heat transfer, the thermal decomposition of the resin, and the resulting mass transfer. These temperatures are then used with mechanical property degradation relations to determine degraded mechanical properties as a function of time. The predicted temperatures and mechanical properties can be used to determine a temperature-dependent coefficient of thermal expansion, and as well to predict thermal deflections. A material model has been developed that adequately represents the elastic-viscoplastic mechanical behavior of laminated FRP composites, and can exhibit all relevant failure modes. Finally, an implementation of this material model within a finite element code, with material properties degraded element-by-element, is used to predict structural behavior.

In addition to the complete description of this process, several other things are included to develop it further. The use of naval composites is described in some detail, along with relevant code requirements. The general behavior of FRP composites in fire is discussed. Following development of each model, relevant parameters for use within the model are provided. For the thermal model, the model
is further characterized statistically—i.e., sensitivity analyses and uncertainty analyses are performed upon it. Validation/verification of the various models is also discussed.
Chapter 1

Introduction

1.1 Use of FRP in Naval Vessels

Fiber reinforced polymer (FRP; e.g. fiberglass) materials have been used in naval structural applications for about sixty years [62, 64, 74]. These materials have been used both in single-skin form and in sandwich panel form, cored with balsa or structural foam. Initially, they were utilized in small personnel boats by the US Navy. With time, the length of FRP naval ships has steadily increased, from under 10 m in length initially to in excess of 70 m in length today. This increased use of FRP composite materials in naval applications is driven by several phenomena.

1.1.1 Benefits of FRP composites

First, these materials offer increased strength-to-weight ratios, allowing for lightweight, and therefore faster and more fuel efficient, craft to be produced. Speed requirements for military and commercial applications are increasing; speeds of more than 60 knots for vessels with a length of more than 40 m are now realistic [62]. In larger vessels, weight is a critically important factor in the speed of the vessel, as a lighter ship displaces less water. Lighter ships are also more fuel efficient, thereby requiring less fuel storage (which further reduces weight). A lower structural weight also allows for increased payloads and increased operational
As well, these materials offer increased corrosion resistance, which substantially reduces maintenance costs vs. traditional steel and aluminum structures. For instance, after more than 20 years of the use of FRP sandwich materials in Swedish naval vessels, with only routine maintenance consisting of inspection and painting, no water absorption or material degradation has been observed [62]. Composites also offer significantly improved resistance to fatigue cracking in comparison to steel or aluminum. FRP sandwich vessels have very good damage tolerance. They also have good repairability, in that damaged sandwich panels have been shown to not absorb water (for instance into their core). As well, after repair, damaged panels have been shown to retain almost all of their original strength [62].

In addition, FRP composites have reduced electromagnetic signatures relative to conventional steel or aluminum materials. This has proven to be a significant advantage in the design of mine counter-measure vessels (MCMVs; minesweepers), as such materials do not trigger magnetic sea mines. In addition, this provides for reduced radar signatures of ships, which are critical in modern stealth naval applications.

Composites are highly customizable materials. By optimally selecting the fiber reinforcement and resin materials, their proportion, the number of fiber layers, and the laminate type and orientation of each layer; materials can be designed with properties tailored to fit a specific application. This level of customization is not possible with traditional metals.

Finally, due to reduced maintenance costs and improved fuel efficiency, the total lifetime cost of a ship, including not only the initial construction material and labor costs, but also life-cycle fuel and maintenance costs, is often lower with FRP composite materials [62].

### 1.1.2 Shortcomings of FRP composites

A primary weakness of composites in naval structures is their increased up-front cost relative to steel or aluminum. However, as previously noted, this cost is often more than offset by reduced lifetime maintenance and fuel costs.
Another major drawback to using composites in larger vessels is a resulting low hull girder stiffness. For instance, per Mäkinen et al., expected hull girder deflections for a 50 m long patrol vessel made of sandwich composite instead of steel increased from 50 m for the steel hull to 150 mm for the composite sandwich hull [62].

A perceived drawback of composite materials relative to traditional metals is their more complex material behavior. This provides a disincentive to using these new materials, as practicing engineers are often more comfortable working with traditional, simpler materials.

When using only glass fiber reinforced polymer (GFRP; fiberglass) materials it is necessary to incorporate conducting materials (e.g. copper mesh) to provide electromagnetic shielding to sensitive electronic components used on the boat, which adds to the construction cost. Carbon fiber reinforced polymer (CFRP) materials provide increased electromagnetic shielding and do not have this drawback. As well, GFRP materials must be routinely painted to prevent UV degradation. However, steel hulls must also be routinely painted to prevent corrosion.

A final critical weakness of composites is their fire behavior, which in addition to being relatively poor, is also poorly understood. The goal of this research is to address this issue; it will be discussed in more detail in Section 1.4 and addressed in subsequent chapters.

1.2 Naval applications

The first naval applications of FRP composites were in small personnel boats (less than 15 m in length) built for the US Navy immediately after the Second World War. By the time of the Vietnam War there were hundreds of personnel boats, river patrol boats, reconnaissance craft and landing craft in service in the US Navy. Composites are currently used as the sole structural material in patrol boats, mine counter-measure vessels (MCMVs), and corvettes. In addition, they are used in the superstructures of small ships, masts for communications ships, piping for destroyers, and fairwaters and casings for submarines [64]. The
US Navy has interest in using composites for both primary and secondary load-bearing structures of ships such as lightweight foundations, deckhouses, masts; for machinery components such as composite piping, valves, centrifugal pumps and heat exchangers [76].

1.2.1 Patrol boats

The first all-GFRP patrol boats were built for the US Navy in the early 1960s. Currently there are over 300 such boats in service. Most GFRP patrol boats are less than 10 m long. They are rarely built longer than about 20 m due to their low hull girder stiffness. For this reason they are used for patrolling inland and coastal waterways, and primarily not for offshore patrol operations [64].

A comparative weight and cost analysis for a 20 m long weight-optimized patrol craft built in aluminum vs. GFRP sandwich showed both a weight and total cost savings of about 10% for the GFRP vessel. The weight savings vs. a steel boat is about 35%. Using recent improvements such as SCRIMP, or using carbon fiber instead of glass, this would be improved even further. It has been estimated that the complete life cycle cost of a composite boat, accounting for maintenance and fuel savings, is about 7% less than for a steel boat [30].

1.2.2 Mine counter-measure vessels

Some of the first naval applications of FRP composites were in mine counter-measure vessels. Such vessels require materials that will not trigger magnetic sea mines, in addition to having high shock resistance. Traditionally wood was used to construct these vessels; however, as the required high quality woods became increasingly expensive after the Second World War, composite materials became more and more cost advantageous [64]. Composites also require reduced maintenance versus wood materials.

The use of composites in MCMVs has driven the creation of ship hull designs that are able to resist local buckling, and provide adequate hull girder stiffness as well as excellent underwater shock resistance. Three hull types are used in MCMVs,
they are framed single-skin, monocoque, and sandwich. The framed single-skin is the most common of these; it consists of transverse frames and longitudinal composite girders that are adhesively bonded in the transverse and longitudinal directions to a pre-laminated GRP hull. The framing system provides the required hull girder stiffness. The monocoque construction does not use a framing system, instead it uses an extremely thick skin (up to 0.15–0.20 m) of GRP. This thickness is needed to obtain the required stiffness and shock resistance without framing. The decks and main bulkheads also contribute to the stiffness of monocoque ships. The third type uses sandwich panels in the hull, wherein the FRP skins are designed to have high stiffness and strength, and the core is designed for high shear resistance and low weight [64].

1.2.3 Corvettes

The longest FRP composite naval ships currently being built are corvettes. In Sweden, the 72 m long YS 2000 or Visby Class is perhaps the most advanced composite naval vessel in the world. It was fabricated using stitched carbon fiber–vinylester sandwich panels with a Divinycell core [21], apparently with glass fiber used as well in various locations [64]. The Visby Class was fabricated via the Seeman composite resin infusion molding process (SCRIMP™) to allow for higher fiber ratios. First the outer laminate skin, together with the core above it, was formed on a vacuum table. This formed panel was then placed on a female mold of the hull and the inner skin was applied as normal [62]. The core was bonded to the skin using Divilette core bedding adhesive [21].

In selecting the laminate design, a first optimization was run to determine the core densities, core thickness, laminate thickness, and lay-up in various locations to minimize weight and cost. Carbon fiber was used in place of the traditional glass, as it allowed for the selection of much thinner laminates—in fact, the number of laminate layers required was reduced to the extent that the reduced labor cost during fabrication offset the increased material costs. The hull weight was reduced by about 30%, to about 20 kg/m$^2$. This provided for a significant increase in range, fuel savings, and performance, and the carbon fiber also provided adequate
electromagnetic shielding for the superstructure [62].

According to the builder, Kockums AB of Sweden, the full-stealth approach (exemplified by the Visby) yields a 99% reduced radar signature versus a conventional design. This leads to it having 1/3 of the susceptibility, or three times higher survivability in a offensive (duel) scenario. Compared to a steel ship with similar equipment, a composite ship has a 90% reduced magnetic signature and can withstand twice the shock factor in an underwater explosion. In a defensive (mine threat) scenario, this leads to a composite ship having roughly four times the survivability of a steel ship. Recoverability after a shock exposure is similar for composite and steel. The builder also claims a 25% reduced average annual total ownership cost for the composite ship due to reduced hull maintenance and replacement costs (as the composite does not corrode), and reduced fuel costs due to the structural weight being reduced by half [66].

1.2.4 Composite superstructures

FRP composites have been utilized in naval ship superstructures for many years. They have been used to construct the deckhouses of patrol boats since the mid-1960s, and to build MCMV superstructures since the early 1970s. The use of FRP composites in naval superstructures provides two primary benefits: the first being reduced corrosion; the second reduced topside weight.

Aluminum has often been used to reduce the weight of naval superstructures. However, aluminum’s high thermal conductivity and significant loss of strength at relatively low temperatures constitute significant drawbacks. The common occurrence of severe fatigue cracking where an aluminum superstructure is welded to a steel hull is another weakness; this has resulted in ships being taken out of service. The “yield” strain of GFRP is about 10 times that of steel, thus the fatigue cracking behavior of FRP composites is expected to be much better [64].

Studies have recommended that superstructures be constructed of single-skin composite panels stiffened with steel framing, or alternatively of FRP composite sandwich panels with top hat stiffeners (having in cross section the characteristic shape of a top hat). Composite superstructures will likely be 15–70% lighter than
steel, though 30% heavier than aluminum. They may be 10–140% more expensive to fabricate, while yielding significantly reduced maintenance costs and improved fuel economy [64].

The French La Fayette Class frigate is the only large warship class currently built with a composite superstructure. The aft portion of the superstructure is constructed of GFRP composite sandwich panels; the ship’s funnels (smokestacks) are also constructed of FRP composites [64].

The US Navy’s next-generation destroyer, the DD(X) Class, is being designed to have an FRP composite deckhouse, with integrated radar and communications system apertures (as opposed to mounting these systems on a separate mast). FRP composites are specified primarily to reduce the structural weight, though reduced radar signature is no doubt a significant consideration [26].

1.2.5 Composite bulkheads

The use of FRP composites in naval bulkheads is being studied. It is expected to yield a weight savings of 20–40% over steel, a lower magnetic signature, better sound damping, and lower heat transmission to adjacent compartments in a fire. However, composite bulkheads would likely be 20–90% more expensive than steel; this increased expense is due in large part to the need for fitting joints at the interface between the composite bulkheads and the surrounding steel structure that provide adequate damage resistance against an internal blast [64].

1.3 Code requirements

1.3.1 Civilian and commercial craft

The United States Coast Guard is the authority having jurisdiction (AHJ) for the commercial marine industry in the United States. In the US, passenger ship construction, as defined in Title 46 of the US Code, is governed by the Code of Federal Regulations (CFR) under Title 46, “Shipping, Chapter I, Coast Guard.” Internationally, the International Maritime Organization (IMO) publishes the In-
ternational Convention for the Safety of Life at Sea (SOLAS) [31].

A guiding principle in these codes since the 1950s has been that a majority of materials on ships are required to be “non-combustible.” A “non-combustible” material is one that “neither burns nor gives off flammable vapors in sufficient quantity for self-ignition when heated to approximately 750 °C” in a vertical cylindrical chamber. This is determined by a standard test procedure, ISO 1182, which is specified in the IMO’s Fire Test Procedures Code [31].

CFR Title 46 currently limits the use of composites to small passenger vessels, life boats and various minor components. The resins in these applications must be approved by the Coast Guard as “fire retardant” per MIL-R-21607. Larger ships are required to use steel or an equivalent non-combustible material [78].

1.3.2 High speed craft

The IMO’s High Speed Craft Code (HSC Code), adopted in 1994, for the first time in recent years allows the use of combustible materials such as composites in the structure of passenger ships. This code is designed for passenger ships on voyages not further than four hours from a place of refuge, or cargo ships not more than eight hours from a place of refuge; and further that do not contain enclosed sleeping berths. In spite of the use of combustible materials, the HSC Code aims to provide a level of safety equivalent to that provided for under SOLAS. It aims to do this via mathematically-based risk management. It also introduces a new definition of “fire-restricting materials,” specifies when these materials are required, and defines test procedures to determine which materials meet this criteria [43, 31].

Mandatory standardized fire tests for commercial ships are specified in both the IMO’s “International Code for Application of Fire Test Procedures” (FTP Code) and the IMO’s “Standard for Qualifying Marine Materials for High Speed Craft as Fire-Restricting Materials,” Resolution MSC.40(64). The IMO’s standard for fire-restricting materials specifies the ISO 9705 “room/corner test” for bulkhead, wall, and ceiling linings; and the ISO 5660 cone calorimeter test method for furniture and other components. These tests measure heat release rate of construction products, and are some of the most modern fire test methods [31].
To ensure the structural integrity of FRP composite bulkheads and decks in fire, the current standard, specified in IMO Resolution MSC.45(65), uses the testing method specified in Resolution A.754(18). In this test a specimen is mounted such that it is supported along only two opposite edges, and then a static load is applied (7.0 kN/m of width for bulkheads, 3.5 kN/m² of area for decks) and deformation measurements are taken. The criteria specified include limiting values for deflection or axial contraction, along with rate of deflection or rate of axial contraction. These criteria are in addition to those specified in Resolution A.754(18). However, this standard has been found to specify static loads which do not adequately represent typical design values. The MARITECH program is a cost shared R&D program jointly funded by the Defense Advanced Research Projects Agency (DARPA) and the marine industry, and one of their efforts aims to address this issue [31].

1.3.3 Military craft

The Military is in the process of developing performance-based standards using commercially available test methods; though waivers may be granted due to mission requirements if materials cannot meet these standards. Two guiding criteria were established for the use of composite systems aboard navy vessels. The first criteria is that the composite not be a fire source, i.e., the material that initiates combustion. The second is that combustion of the composite should be delayed until the crew is able to respond to the primary fire source [76].

The use of composites inside naval submarines is covered by MIL-STD-2031 (SH), “Fire and Toxicity Test Methods and Qualification Procedure for Composite Material Systems Used in Hull, Machinery, and Structural Applications Inside Naval Submarines.” This standard provides test methods and requirements for flame spread, specific optical density of gases, heat release and ignitability, etc. These include: oxygen index, ASTM D-2863 modified; smoke obscuration, ASTM E-662; flame spread index, ASTM E-162; cone calorimeter heat release rates, ASTM E-1354; resistance to flame penetration, burn-through test; flashover potential, US Navy quarter scale test; et cetera [78, 76].

Per Sorathia et al., as of 2001 there was no specific fire-related standard for
composite structures on surface ships. Guidance and requirements have been provided by NAVSEA 05L4 on a case-by-case basis. The US Navy currently recommends screening potential composite materials using small-scale tests (i.e. cone calorimeter, ASTM E-1354; and lateral ignition flame spread test, ASTM E-1321) and analysis tools. Full-scale testing using the UL 1709 fire exposure is then recommended using the selected material to verify that fire growth, visibility, smoke toxicity, fire resistance, and structural integrity are acceptable [76].

1.4 Fire Behavior of Composites

1.4.1 FRP composite materials

Fiber reinforced polymer composites are composed of fibers which have been impregnated with a polymer matrix and allowed to set. These materials are particularly effective due to the fact that long thin fibers of various materials can be made much stiffer and stronger than the same material in bulk form. Individual fibers (with width on the scale of a single crystal of the material) may be manufactured with a more perfect structure than a bulk material, and with fewer internal defects [46].

FRP composites are commonly utilized in the form of a laminate. The fibers within a layer are generally first formed into a fabric using techniques originally developed for the production of textiles—i.e. they are woven, stitched, or knitted together. These layers are then impregnated with matrix, with each flat layer of fibers and matrix forming a single lamina.

The matrix serves a critical mechanical purpose in the composite: it supports the individual fibers, protects them, and transfers load among and between them. Per Jones, matrix materials may be polymers, metals, ceramics, or carbon; listed in order of increasing cost and thermal resistance [46]. For the construction of large naval structures, materials are limited in practice to polymers. Though these materials are generally available at a reasonable cost, they also have relatively poor thermal behavior; again the goal of this research is to characterize and address this behavior.
A polymer is a very long molecule consisting of repeating units connected by covalent chemical bonds. The repeating unit is called a monomer. Commonly-used matrix polymers (plastics) include polyesters, vinylesters, and epoxies; these are organic polymers, i.e. they have carbon-based monomers. Generally, polyesters are the least expensive and have the poorest mechanical properties, epoxies are most expensive and have the best mechanical properties, and the cost and properties of vinylester lie in-between the two. Vinylester is also more resistant to corrosion than polyester resin. Vinylester was chosen for use in the Visby Class corvette, for instance, and its chemistry will be discussed in more detail.

1.4.2 Vinylester polymer

The chemical structure of vinylester resin is widely available, and will not be discussed here. For more information, see for instance [54]. However, the thermal behavior of e-glass vinylester composites will be discussed in detail in the following sections.

1.4.3 Response of polymers to increasing temperature

Differential scanning calorimetry (DSC) is used to understand changes in polymer state upon exposure to heat. DSC involves two identical enclosed pans—one empty, and one containing a sample of the polymer of interest. Each pan is heated at a constant rate of temperature change, and the amount of heat input required to raise the temperature of both pans is recorded with time. From this data, the heat required to raise the temperature of the polymer sample itself, with the effects of the pan and air removed, can be obtained as the difference between the two values. A plot of this data, heat flow required vs. temperature, represents an apparent specific heat capacity, or heat required to raise the temperature one degree Celsius per kilogram, as a function of temperature [69].

A general polymer will be partially amorphous and partially crystalline. As it is heated, it will reach a glass transition temperature \( T_g \). At this temperature, the amorphous portion of the polymer will leave its glassy state and change into
a rubbery state. This will be visible on a DSC curve as an permanent increase
in apparent specific heat capacity. Upon further heating, if the polymer could
crystallize, it would reach its crystallization temperature $T_c$, at which point the
amorphous portion of the polymer would become crystalline. This transition in-
volves the release of heat, and is visible as a temporary reduction in the apparent
specific heat capacity of the polymer. Finally, the polymer would reach its melting
temperature, at which point the crystalline polymer would melt. This requires
additional heat, and is visible in the DSC plot as a temporary increase in the
apparent specific heat capacity [69]. It is important to note that these described
effects are phase transitions within the polymer, and do not involve the physical
degradation of the polymer due to pyrolysis. However, pyrolysis would also be
visible on the DSC result, and must be considered separately.

Thermogravimetric analysis (TGA) is used to determine the thermal decom-
position behavior of a polymer. TGA involves a single pan with a polymer sample
placed upon it. The pan and sample are again heated at a constant rate of temper-
ature change. However, here the mass of the sample is measured as a function of
increasing temperature. Thus, as the organic polymer pyrolizes to produce gases
and carbonaceous char, the mass that is lost to gas production is measured.

DSC data for a woven e-glass/Derakane 510A vinylester composite ground into
a powder and placed in an inert (100% nitrogen) environment is presented in
Figure 1.1. TGA data for the same e-glass vinylester composite ground into a
powder and placed in an inert (100% argon) environment is presented in Figure 1.2.
These data were obtained by Brian Lattimer et al. at Hughes Associates, and are
available in the literature [50].

The TGA plot shows that about 72% of the powder mass remains after the de-
composition reaction is completed. These samples contained about 30% by weight
of resin [50], so clearly vinylester resin decomposes almost entirely into gases, leav-
ing almost no carbonaceous char. The decomposition reaction at a 16 °C/min
heating rate is seen to occur between about 320 °C and 420 °C. Slower (faster)
heating rates lead to pyrolysis at slightly lower (higher) temperatures.

The DSC result for the powder at a 16 °C/min heating rate shows a clear perma-
Figure 1.1: DSC result (apparent specific heat capacity), normalized with respect to the initial mass of the sample [50]

Figure 1.2: TGA result (mass fraction) [50]
nent increase in apparent specific heat capacity between about 120 °C and 140 °C. From this one could estimate a value for $T_g$ of 130 °C. The next clear change in the apparent specific heat capacity occurs at about 320 °C. However, it is known from the TGA result that this marks the beginning of the pyrolytic decomposition of the polymer into gases and char. Thus no further phase transitions are observed.

An inert environment is provided in both experiments because the in situ decomposition behavior is desired. The events which occur in a burning polymer within an FRP composite panel include first the application of heat to thermally degrade, or pyrolyze, the solid polymer to low–molecular weight volatile fuel and nonvolatile solid char. The following assumes a reverse-smolder situation, in which these low–molecular weight gases are assumed to flow outward from the panel, or in the opposite direction as the heat flow. Upon reaching the boundary with the outside environment, these volatile thermal degradation products mix with atmospheric oxygen and may ignite. A minor fraction of any combustion energy is returned to the polymer surface via convection and radiation; a majority is lost to the environment [61]. Combustion only occurs between the pyrolysis products at the boundary and oxygen from the external environment. To analyze the pyrolytic decomposition of the solid resin to produce gas, we must replicate the internal situation at a location removed from the combustion zone. At this internal location, pyrolysis gases which are being produced are flowing outward, and have yet to reach the external boundary at which oxygen is present. Thus the pyrolytic decomposition of the polymer occurs in an inert environment; the combustion of the product gases is a separate issue. For a more detailed description of the pyrolytic decomposition of polymers, see [61].

This sheds light on an apparent dichotomy with regard to the fire properties of FRP composites. On the one hand, their fire behavior is understood to be very poor. For instance, one Navy researcher has concluded that “97 °C represents the upper threshold of operating temperatures for unprotected glass-reinforced vinylester load bearing composite structures [75].” On the other hand, these same materials which are thought to have poor fire behavior in structural applications are commonly chosen for use in applications such as ablatively shielding spacecraft.
from the intense heat of atmospheric re-entry. Commonly used ablative materials include glass or carbon fiber–epoxy composites [88]. How can the same material which has such poor structural behavior when exposed to relatively mild temperatures be the material of choice in applications which require exposure to extremely high temperatures?

On the one hand, its relatively low glass transition temperature causes the resin to lose its strength at a relatively low temperature. On the other hand, there are several properties of composites which are quite beneficial in high-temperature applications, and which lead to their use as ablative materials. The thermal conductivity of a typical composite, between 0.1 and 0.3 W/m·K, is similar to the value for wood, and is less than one percent of that for steel, and an even smaller fraction of the value for aluminum [50]. Furthermore, so long as a reverse-smoldering situation is maintained, the pyrolosis gases which are produced travel in the opposite direction as the heat flux. As these gases leave the panel, they carry with them heat, cooling the panel. Also, as these gases exit the panel surface, they partially block the convective heat flux from entering the panel [88]. The reverse-smoldering situation also provides for the pyrolysis of the polymer to occur in the absence of oxygen. This leads to an endothermic degradation reaction, wherein heat is absorbed, further cooling the panel. Note that were gases able to flow through the panel in the direction of the heat flow (forward-smoldering situation), oxygen might be present, and this reaction might become exothermic, leading to a more rapid temperature rise. So one might conclude that while the mechanical behavior of a composite material exposed to fire is quite poor, the thermal behavior of the material, especially in a reverse-smoldering situation (which is most common), is actually very good.

1.4.4 Further issues

The preceding description of the fire behavior of an e-glass vinylester composite focuses on its thermal and mechanical behavior. However, there are other critical issues in the fire behavior of FRP composite structures. These include their habitability during a fire event, the growth rate of any fire, and the ease of
extinguishment of said fire. The habitability of a composite structure in fire is determined by its flame, smoke, and toxicity (FST) behavior—i.e., do any of these three items preclude the environment from being habitable, at least during such time as required for the fire to be extinguished. The fire growth rate is largely determined by the heat release rate (HRR) of the burning material. Also of interest is the possibility of the occurrence of flashover, which may be demonstrated in a room-corner burn test. All three of these items are critically important to the fire behavior of FRP composites, but are outside of the scope of the current research and will not be discussed herein. For a discussion of these issues see for instance [77].
Chapter 2

Analytical method

2.1 Introduction

The single greatest impediment to the use of FRP composites in the design and construction of advanced ship structures is their susceptibility to degradation during exposure to the elevated temperatures of a fire. Per Caplan et al., “the critical issue in surface ship fires is the residual strength of structures at elevated temperatures for a period of 30–60 minutes,” in addition to their flame, smoke, and toxicity (FST) behavior [14]. Thus if the use of such advanced materials in ships is to succeed, the behavior of FRP composite structural members exposed to fire must be understood and quantified within a design framework.

To this end, one of the stated goals of the ONR is to develop “analytical models that can predict the structural behavior of composites during fire as well as the post-fire mechanical performance.” In particular, “the methodology will require integration of thermal distribution (fire), viscoelastic behavior (polymer matrix), and thermo-mechanical (structural) mathematical models into an existing finite element analysis model (ABAQUS). The models will be verified through small and large scale fire tests [14].”

In this chapter, the overall methodology used to model the behavior of FRP composite sandwich structures upon exposure to fire is introduced. The individual steps will be described in a “black box” sense, in that only the required input parameters and the resulting output data will be identified here. The individual
Thermal model

Property degradation

Thermal strains

Material model

Structural model

Figure 2.1: Flow chart for analytical method. Predicted temperatures determine degraded mechanical properties and thermal strains. Degraded mechanical properties affect coefficient of thermal expansion (used in thermal strain calculation). Degraded mechanical properties and thermal strains are imposed upon material model. Material model is implemented in finite element structural model. At a later date, the material model may be coupled with the thermal model, wherein the current stress state would influence the material porosity in a volume-changing thermal model (accounting for material expansion/pressurization).

steps will be detailed in subsequent chapters, as referenced herein. The overall methodology is derived from that called for by the ONR as just quoted. It includes a coupling of several models—a thermal model to determine the thermal decomposition behavior of the composite in fire; a model of the degradation of the composite’s mechanical properties with increased temperature, as a result of its phase transitions as described in Section 1.4.3; a description of the thermal strains that result from the current thermal and mechanical property state; a model of the elastic-viscoplastic material behavior of the laminated composite, which incorporates the degraded mechanical properties and thermal strains, and is implemented into a finite element code; and structural finite element models, which model whole structures, using the material model just described, degraded as per the predicted temperatures and degradation models, and with thermal strains imposed as appropriate. This process is described in Figure 2.1.
2.2 Thermal model

A one-dimensional thermal model from the literature has been numerically implemented to predict the temperature variation within the panel due to fire exposure. This model requires several material parameters to be defined. These include thermophysical constants, which are quite strongly temperature-dependent—viz the thermal conductivity of the virgin composite and char; and the specific heat capacity of virgin composite, char, and pyrolysis gases (at constant pressure). Also the mass densities of the virgin composite and char, and as well the heat of decomposition of the composite are needed. The decomposition reaction is represented as an Arrhenius reaction of arbitrary order; requiring that a pre-exponential constant, activation energy, and reaction order be specified. Finally, the heat-transfer properties of the boundary must be specified, viz the convection heat transfer coefficient at the hot and cold faces, and the emissivity of the hot and cold faces. Since the thermophysical constants are strongly temperature-dependent, these are specified as temperature-dependent functions (with slope and intercept, as defined in Chapter 3). Thus twenty material property input parameter values are required. As well, initial conditions (initial temperature) and boundary conditions (flame temperature or incident heat flux at hot face, ambient temperature at cold face) must be specified. The thermal model, with these material parameters, initial and boundary conditions provided, results in predicted temperatures with time throughout the panel, as in for instance Figure 2.2.

2.3 Property degradation model

As discussed in Section 1.4.3, as the resin in a composite approaches its glass-transition temperature, it transitions from a glassy (stiff) to a rubbery (pliable) state. This change is not abrupt, but gradual. The resulting fraction of various virgin material mechanical properties as a function of temperature has been determined, for instance as seen in Figure 2.3.

So the thermal model temperature values are taken, and passed through this model of mechanical property degradation as a function of temperature, to result
Figure 2.2: Predicted temperature evolution with time

Figure 2.3: Fraction of virgin mechanical properties (both elastic constants and shear constants) as a function of temperature for e-glass/vinylester FRP, together with fraction of elastic constants for various core materials in a prediction of the varying mechanical property gradation within the panel as a function of time. This is discussed in more detail in Chapter 8.
2.4 Thermal strains

From the degraded elastic modulus, an estimate of the degraded coefficient of thermal expansion of the composite may be obtained throughout the panel. This coefficient of thermal expansion gradation, together with the temperature gradation and elastic modulus gradation, may be used in a separate model to predict the thermal deflections of the panel, for instance as in Figure 2.4.

![Maximum thermal deflection (5/8" insul.)](chart)

Figure 2.4: Predicted thermal deflections as a function of time.

If deflections are small and higher-order effects are minimal, one could linearly superimpose the thermal deflection, calculated in this manner, with the mechanical deflection (calculated without thermal strains). This method has the disadvantage of neglecting higher-order effects. However, the separate solution of the thermal deflection problem does not involve such a coarse discretization as the finite element structural solution, and so its estimation of the thermal deflection alone is likely to be significantly more accurate. This is discussed in more detail in Chapter 6.

Alternatively, the thermal strains (a function of the coefficient of thermal expansion of the material and the temperature change) may be directly implemented within the material model. This allows for higher-order effects to be accounted for directly. However, it also restricts the expression of the thermal strains to be as
coarse as the structural discretization.

2.5 Material model

According to Fleck, “evidence is accruing that the dominant mechanism of compressive failure in polymer-matrix composites is plastic microbuckling. The compressive strength is controlled by fiber misalignment together with plastic shear deformation in the matrix.” [22] Thus a material model must be developed that will demonstrate shear kinking in the presence of a fiber misalignment, in addition to skin wrinkling and global buckling failure modes. Such a model is developed based upon one commonly used for crystal plasticity. In crystal plasticity, a dislocation is formed along a slip plane between two layers of molecules arranged in a crystalline lattice, and then slip occurs along this slip plane. In the current application, slip occurs due to interlaminar shear, as the fiber laminae slip alongside each other along the slip plane (oriented parallel to the laminae, or in other words parallel to any fiber misalignments). In crystal plasticity, the resistance to slip is governed by intermolecular forces, while in the case of a compressively-loaded FRP laminated composite, the resistance to slip is governed by the shear strength of the matrix resin. Thus by using this crystal plasticity–based model in the current application, the mechanics of interlaminar shear which drive this plastic microbuckling failure mode may be adequately represented. This model is discussed in more detail in Chapter 7.

The material model requires as input the elastic constants, which may or may not be thermally degraded. The shear strain rate is defined using several parameters, including a reference shear strain rate and a strain rate sensitivity exponent. Other parameters include an initial flow stress, a saturation flow stress, and a hardness modulus (each of which may be degraded according to a shear property degradation relation, for instance as depicted in Figure 2.3).
2.6 Structural model

This material model is then used in a finite element structural model to determine the mechanical behavior of the overall structure. For each element, the material properties are uniform, and taken to be those corresponding to the temperature at the element midpoint. This requires that the structural geometry and boundary conditions be specified. It results in the predicted structural behavior, which may take the form of predicted deflections, predicted failure modes, or predicted time-to-failure. The structural solution may be solved in time in two ways: the first is to observe the time behavior in snapshots, implementing the degraded material properties at a given instant and then solving for the structural state at that instant (via dynamic relaxation). The second is to degrade the properties as the simulation progresses, and solve quasistatically. This modelling is discussed in more detail in Chapter 9.

If a quasistatic solution is used, with the material properties being degraded as the simulation progresses, the simulation will predict failure load, time-to-failure, the initial failure mode, and any subsequent failure modes which may be brought upon by the initial failure mode. For instance, plastic microbuckling might be observed, which might then lead to a skin wrinkling failure. If the problem is solved via dynamic relaxation, the simulation will predict failure load, time-to-failure, the initial failure mode, and perhaps subsequent failure modes. The dynamic relaxation solution will reveal a complete picture of the sequence of events that occur after failure is initiated only if the snapshot at the failure load is simulated, and if the problem solution is quasistatic—as judged, for instance, by ensuring that the kinetic energy of the system remains small as a fraction of its total energy—i.e., less than 5% or so.

An example of the predicted behavior that is available via the dynamic relaxation solution is given in Figure 2.5.

This figure shows the deflection due to the structural behavior; it then shows the deflection due to the structural behavior plus the thermal deflections (from the separate thermal deflection model) combined linearly. This prediction does not, therefore, account for higher-order effects. A similar example is described in more
Out-of-plane Total (and Mechanical Only) Deflections with Time

- 2 kip/ft, 5/8" insul.
- 3 kip/ft, 5/8" insul.
- 2 kip/ft, 1-1/4" insul.
- 3 kip/ft, 1-1/4" insul.

Figure 2.5: Predicted structural deflection with time
detail in Chapter 10.
Chapter 3

Thermal model

In this chapter, a model for the thermal response of an FRP composite sandwich panel is developed. The chapter begins with a review of the relevant literature; it then proceeds into the development of a model built upon this foundation.

3.1 Review of the literature

Several transport models for the thermal degradation of charring solids have been developed. A majority of these models have been derived for cellulosic materials (i.e. wood). The number of models which have been derived for FRP composites is significantly smaller. Many of the models derived for composites have been intended to predict the behavior of charring ablative materials, for instance as would be used to shield a spacecraft from the intense heat of atmospheric re-entry. A more complete review of all of these models is available in the literature [19]. A brief summary of relevant models developed for FRP composites follows.

Of the models derived for FRP composites, the model by Henderson, Wiebelt, and Tant seems to have been among the first, and among the most influential [37]. This one-dimensional model, published in 1985, was derived in a manner parallel to similar models for cellulosic solids. It assumes no pressurization, no volumetric expansion, and that thermal equilibrium exists between gases and solid. It was solved using a finite difference technique. The model was expanded in 1987 to account for pressurization due to the accumulation of pyrolysis gases, and as well
for volumetric expansion [38]. In 1991, the model was modified still further to relax the assumption of local thermal equilibrium between the product gases and the porous solid [23].

Also in 1991, Milke and Vizzini published a model for the three-dimensional heat transfer problem (Fourier’s law) only, and did not consider the decomposition of the resin, etc. [63]

In 1992, Sullivan and Salamon published a model for the thermal and mechanical response of FRP composite materials to fire, based in part on the work of Henderson et al. The model is three-dimensional, though it assumes transverse isotropy [85]. The model brings the material’s stress state into the thermal solution, as it affects the thermochemical expansion which results from the pressurization due to production of pyrolysis gases. The model is solved in the physical domain via a finite element method, and in the time domain via a finite difference solution. Two subsequent papers published provide validation and example applications of this model [86, 84].

In 1995, Gibson et al. published a paper providing and applying a one-dimensional thermal model, apparently taken from previous papers for cellulosic materials and as well from the work of Sullivan, and solved via finite difference methods [29]. In 1997; Looyeh, Bettess, and Gibson published a paper which more fully develops the model provided in Gibson’s 1995 paper; and solves it numerically using a finite element solution [59].

Also in 1997, a one-dimensional model was developed by Shih and Cheung, accounting for the resin decomposition, temperature-dependent material properties, lack of thermal equilibrium, pressurization, and volumetric expansion. The model is solved via a finite volume technique [73].

In 1998, Looyeh and Bettess expanded their earlier model to account for temperature-dependent material properties, and the existence of voids at the interface between the sandwich panel skins and core [58]. Their numerical implementation of this model was improved in 2001 [60].

Also in 1998 Torre, Kenny, and Maffezzoli derived a one dimensional model [89]. The model allows for a lack of thermal equilibrium, but assumes no expansion nor
pressurization takes place. It allows for multiple materials to be present in the composite, each of which has its own degradation reaction equation (useful in ablative materials). The model is solved using a finite difference method.

In 1999, Looyeh published his doctoral dissertation. In this he expands their previous model into two dimensions [56]. He also accounts for pressurization within the panel due to the accumulation of pyrolysis gases. The application of this model to joined FRP composite panels was discussed in 2001 [57].

In 1999, Staggs developed a one-dimensional thermal model for a composite of polymer resin, and various inert fillers [80]. This model assumes no pressurization, and is solved via an implicit finite difference method. Staggs demonstrates in a separate paper that the assumption of a first-order reaction equation doesn’t introduce significant error [79]. In 2000, Staggs expanded this model to account for volume changes [81].

In 2000 Leach et al. published a one-dimensional forward smoldering model [51]. All of the models discussed previously are backward smoldering; that is the pyrolysis gases flow in the opposite direction as the heat. This insures that the polymer degrades in an inert atmosphere, and thus that the degradation reaction is endothermic, cooling the panel. In the forward smoldering model, the gases move in the same direction as the heat, allowing for the possibility that the decomposition reaction may take place in an oxygen-rich atmosphere. Thus the reaction may be exothermic, leading to a vastly different (and more severe) thermal situation. The model is solved via a finite difference solution.

Also in 2000, Zhou and Fernandez-Pello published a model for the pyrolysis and ignition delay of composite materials [93]. As pyrolysis gases produced endothermically in an inert environment reach oxygen-rich air at the panel exterior, they may ignite. This model predicts the time-to-ignition for a given heat flux via the control volume method.
3.2 Introduction

The goal of the current work is to model the mechanical behavior of FRP composite sandwich structures exposed to fire. The first step in such a process is to develop a predictive model to determine the temperature profiles that will likely exist within various panels as a function of time and heat exposure.

This model will describe in particular the initial heating of the composite with fire exposure (via heat transfer relations). As the temperature increases, it will describe the endothermic decomposition of the matrix resin into gaseous products, which serves to cool the panel. Beyond this, with the matrix resin all converted into gaseous products, the problem is again governed by heat transfer relations.

In this chapter, the partial differential equation (PDE) model will be developed, with reference to the literature. The issue of the proper formulation of the finite element discretization will be explored, with particular attention devoted to the formulation of the time stepping and update of the various quantities in the model.

The convergence of the model will be demonstrated, both spatially and in time. First a brief review of the PDEs is provided, including a discussion of the boundary conditions. Then the space-discrete model via the weighted residual equation is derived, and the issue of time discretization is discussed. A fully implicit time stepping scheme based upon the Crank–Nicolson stencil for both the temperatures as the primary variables, and also for the mass density as the constitutive variable, is proposed. The paper is concluded with a discussion of a validation problem.

Although a comprehensive modelling effort directed at the problem of sandwich panels is presented, in practice this entails concentration on the behavior of the hot laminate skin of the panel as the most relevant part of the model. The core is assumed not to decompose, and the cold skin is modelled in precisely the same manner as the hot one.

3.3 The PDE model

The PDE model of the transient heat conduction problem with chemical decomposition is essentially the one derived by Henderson, Wiebelt, and Tant [37].
The model is summarized very briefly herein for the readers’ convenience.

The composite panel considered here is assumed to be loaded by a heat flux (or prescribed temperature) that is essentially uniform in the plane of the panel, and hence the model is strictly one-dimensional, extending through the thickness of the panel only. The modelling treated in this work is applicable to single skin composite plates, or to sandwich composite plates. Figure 3.1 describes this situation.

Figure 3.1: Sketch of the panel.

The material of the laminate skin of the panel consists of at least two phases: solid phase (mixture of resin matrix, reinforcement fibers, and residues of the decomposition reactions), and gas phase (products of the decomposition reaction, and air).

The main assumption is that no solid-phase material flows into or out of a control volume fixed in space. Of course, solid phase is lost as it is converted into gas. The gas simply flows through the control volume—it does not accumulate. Hence, there is no volumetric expansion, and no distinction between Lagrangian and Eulerian modelling needs to be made.

Consider a control volume, viz. the interval $x$ to $x + \Delta x$ in the direction of the thickness of the panel. The balance of energy in the volume:

$$\Delta x \frac{dU}{dt} = q(x) - q(x + \Delta x) + (\dot{m}_g h_g)(x) - (\dot{m}_g h_g)(x + \Delta x) + \bar{s} \Delta x \quad (3.1)$$
which yields in the limit of $\Delta x \to 0$

$$
\frac{dU}{dt} = -\frac{\partial q}{\partial x} - \frac{\partial}{\partial x}(\hat{m}_g h_g) + \hat{s}, \quad (3.2)
$$

where

- $U$ = internal energy density per unit volume [J m$^{-3}$]
- $q$ = heat flux [W m$^{-2}$]
- $\hat{m}_g$ = mass flux of gas [kg s$^{-1}$ m$^{-2}$]
- $h_g$ = gas enthalpy [J kg$^{-1}$]
- $\hat{s}$ = total rate of heat generation per unit volume [W m$^{-3}$]

Note that the assumption of the absence of deformation also excludes from consideration a receding exposed surface.

Fourier’s constitutive equation for $q$ is assumed,

$$
q = -k \frac{\partial T}{\partial x}, \quad (3.3)
$$

where

- $T$ = absolute temperature [K]
- $k$ = thermal conductivity [W m$^{-1}$ K$^{-1}$].

The thermal conductivity $k$ generally depends on the temperature, $k = k(T)$, both directly and also indirectly through the composition of the solid phase (more on this later). Thus,

$$
\frac{dU}{dt} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) - \frac{\partial}{\partial x}(\hat{m}_g h_g) + \hat{s} \quad (3.4)
$$

The internal energy density of the mixture of fibers, resin, and decomposing resin is assumed to be proportional to the enthalpy $h$ (no volume change!): $U = \rho h$. Therefore,

$$
\frac{dU}{dt} = \frac{\partial}{\partial t} (\rho h) = \frac{\partial \rho}{\partial t} h + \rho \frac{\partial h}{\partial t} = \frac{\partial \rho}{\partial t} h + \rho \frac{\partial h}{\partial T} \frac{\partial T}{\partial t} \quad (3.5)
$$

where

- $\rho$ = mass density of the solid phase [kg m$^{-3}$]
Thus,
\[
\frac{dU}{dt} = \frac{\partial \rho}{\partial t} h + \rho c_p \frac{\partial T}{\partial t}
\]  
(3.6)

where
\[c_p = \text{specific heat [J kg}^{-1}\text{K}^{-1}]\].

The convective term may be expanded as,
\[-\frac{\partial}{\partial x} (\dot{m}_g h_g) = -\frac{\partial \dot{m}_g}{\partial x} h_g - \dot{m}_g \frac{\partial h_g}{\partial x} .\]

Since the gas does not accumulate in the control volume, the mass balance of the gas reads
\[\dot{m}_g(x + \Delta x) - \dot{m}_g(x) = (\text{rate of production of gas}) \times \Delta x\]

The rate of gas production may be expressed as the negative rate of change of the mass density of the solid phase,
\[\frac{\partial \dot{m}_g}{\partial x} = -\frac{\partial \rho}{\partial t}\]

where \(\rho\) is the mass density of the solid phase. Further, assume the gas enthalpy approximately as \(h_g \approx c_{pg} T\), and the enthalpy of the solid phase as \(h = c_p T\). Collecting all terms gives
\[\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) - \frac{\partial \rho}{\partial t} (h - h_g) - \dot{m}_g c_{pg} \frac{\partial T}{\partial x} + \tilde{s} .\]  
(3.7)

The source term, \(\tilde{s}\), could include a number of exothermic or endothermic reactions. In particular, in this work it shall include the heat of the matrix decomposition reaction. Thus,
\[\tilde{s} = -Q \frac{\partial \rho}{\partial t} + \ldots ,\]  
(3.8)

where
\[Q = \text{heat of decomposition, positive for exothermic reactions [J kg}^{-1}]\].
3.3.1 Composition of the solid phase

It is assumed herein that the composite undergoes a single chemical reaction, the decomposition of the resin matrix into gases. The solid phase needs to be treated as a mixture that consists of the virgin (intact) material and the residue of the resin decomposition reaction. It is assumed for vinylester or polyester resins that the decomposition reaction consumes all of the resin, and hence that the residue consists of simply the fiber reinforcement. On the other hand, for phenolic resins the char composition is more complicated.

In agreement with Reference [37] (but not with the models of References [59, 58], where the mixing is treated on the level of mass densities of the resin and the fiber reinforcement) the composition of the solid phase is described using a mixture equation with $F$ being the fraction of the current mass density of the resin in the solid phase and the initial mass density of the resin in the virgin material.

\[ F = \frac{\rho - \rho_{ch}}{\rho_v - \rho_{ch}} \]  

(3.9)

Here

- $\rho_{ch}$ = mass density of the solid phase at the completion of the decomposition reaction [kg m$^{-3}$];
- $\rho_v$ = mass density of the intact (virgin) material [kg m$^{-3}$].

Thus, the mass density of the mixture may be expressed as

\[ \rho = F\rho_v + (1 - F)\rho_{ch} \]  

(3.10)

In the absence of measured material data the virgin material and char mass densities may be estimated from the properties of the resin and fiber reinforcement alone. A more substantial discussion follows below.

It is assumed in this work that thermal properties of the solid phase may be estimated using mixture equations analogous to (3.10)

\[ k = Fk_v + (1 - F)k_{ch} \]  

(3.11)

\[ c_p = Fc_{pv} + (1 - F)c_{pch} \]  

(3.12)
where

\[ k_{ch} = \text{thermal conductivity of the solid phase at the completion of the decomposition reaction [W m}^{-1}\text{K}^{-1}] ; \]
\[ k_v = \text{thermal conductivity of the intact (virgin) material [W m}^{-1}\text{K}^{-1}] . \]
\[ c_{pch} = \text{specific heat of the solid phase at the completion of the decomposition reaction [J kg}^{-1}\text{K}^{-1}] ; \]
\[ c_{pv} = \text{specific heat of the intact (virgin) material [J kg}^{-1}\text{K}^{-1}] . \]

This is quite reasonable for the specific heat, but less so for the thermal conductivity. Formula (3.10) is in fact a bound on the actual thermal conductivity corresponding to an arrangement of constituents parallel to the direction of heat flow (see Reference [87], and also the discussion in Reference [82]).

The decomposition reaction describes the rate of mass density change by an \( n \text{th} \) order Arrhenius equation (written in terms of the mass density because the volume is fixed)

\[
\frac{\partial \rho}{\partial t} = -A \rho_v \left( \frac{\rho - \rho_{ch}}{\rho_v} \right)^n \exp \left( -\frac{E_a}{RT} \right)
\]  (3.13)

where

\[ A = \text{pre-exponential factor [s}^{-1}] \]
\[ E_a = \text{activation energy [J kmol}^{-1}] \]
\[ R = \text{gas constant [8,314 J kmol}^{-1}\text{K}^{-1}] \]
\[ n = \text{order of the reaction [ND]} \]

This equation may be rewritten in terms of the fraction \( F \) as

\[
\frac{\partial F}{\partial t} = -A \left( \frac{\rho_v - \rho_{ch}}{\rho_v} \right)^{n-1} \exp \left( -\frac{E_a}{RT} \right) F^n
\]  (3.14)

from which one may express

\[
\frac{\partial \rho}{\partial t} = \frac{\partial F}{\partial t} (\rho_v - \rho_{ch}) .
\]  (3.15)
3.3.2 Summary of the balance equations

To summarize, one has the balance equations

\[
\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) - \frac{\partial \rho}{\partial t} (h - h_g) - \dot{m}_g c_{pg} \frac{\partial T}{\partial x} - Q \frac{\partial \rho}{\partial t} \]

\[
\frac{\partial \dot{m}_g}{\partial x} = -\frac{\partial \rho}{\partial t} \tag{3.16}
\]

with unknowns \( T, \rho, \) and \( \dot{m}_g \). However, boundary conditions for the gas mass flux will help to eliminate the last quantity, and one may show that the mass density \( \rho \) may be treated as a constitutive quantity. Thus, one may reduce the above system into a single partial differential equation for the unknown function \( T \).

3.3.3 Initial conditions

\[
\rho (0) = \rho_v \\
T (0) = T_{ini} \tag{3.17}
\]

where

\[
T_{ini} = \text{ initial temperature [K]}. 
\]

3.3.4 Boundary conditions

**Hot face**: A combination of common boundary conditions may be prescribed as

\[
q''(t, 0) = \epsilon_h \bar{q}''(t) - k_{sh} (T_{fl}(t) - T(t, 0)) + \epsilon_h \sigma ((T_{fl}(t))^4 - (T(t, 0))^4) \tag{3.18}
\]

where

\[
\epsilon_h = \text{ emissivity of hot face} \\
\bar{q}'' = \text{ prescribed heat flux [W m}^{-2}]; \text{ notice that } \bar{q}'' \text{ is assumed not to be functionally dependent on } T_{fl} \\
\sigma = \text{ Stefan-Boltzmann constant, } \sigma = 5.67 \times 10^{-8} \text{ [W m}^{-2} \text{ K}^{-4}] \\
k_{sh} = \text{ surface heat transfer coefficient on the hot face [W m}^{-2} \text{K}^{-1}]
\]
\[ T_{fl} = \text{temperature of the flame (oven) [K]} \]

Notice that \( k_{sh} \) may be used as a penalty parameter to enforce prescribed surface temperature, \( T(t, 0) = T_{fl}(t) \). Also, note that \( k_s \) is used to represent the heat transfer coefficient, and should not be confused with \( k \), which represents the thermal conductivity. Note also that the user is responsible for defining the thermal boundary condition as some combination of prescribed radiant heat flux, or temperature record—a furnace temperature record will lead to the convection and radiation terms being activated, while the prescribed heat flux will not.

**Cold face:**

\[ q''(t, l) = k_{sc} (T(t, l) - T_a(t)) + \epsilon_c \sigma ((T(t, l))^4 - (T_a(t))^4) \tag{3.19} \]

where
\[
\begin{align*}
  k_{sc} & = \text{surface heat transfer coefficient on the cold surface [W m}^{-2} \text{K}^{-1}], \\
  T_a & = \text{ambient temperature on the cold surface [K]}, \\
  \epsilon_c & = \text{emissivity of cold face}.
\end{align*}
\]

**Gas mass flux:** Furthermore, it is assumed that no decomposition gases exit through the cold surface, which is a reasonable assumption for the early stages of the decomposition, especially for sandwich panels. Thus,

\[ \dot{m}_g(t, l) = 0 . \tag{3.20} \]

Note that this boundary condition makes it possible to eliminate the gas mass flux from the system (3.16) by integrating

\[ \dot{m}_g(l) - \dot{m}_g(x) = \int_l^l \frac{\partial \dot{m}_g}{\partial x} dx = - \int_x^l \frac{\partial \rho}{\partial t} dx = \int_l x \frac{\partial \rho}{\partial t} dx = 0 \tag{3.21} \]

Hence, we obtain the system (3.16) in residual form

\[ r(x, t) = \rho c_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial \rho}{\partial t} (h - h_g) - \left( \int_x^l \frac{\partial \rho}{\partial t} dx \right) c_{pg} \frac{\partial T}{\partial x} + Q \frac{\partial \rho}{\partial t} = 0 \tag{3.22} \]
for the unknown function $T$ in variables $x$ and $t$. The mass density is a dependent of the unknown $T$, and is driven by the evolution equation (3.13). Equation (3.22) is accompanied by the initial conditions (3.17), and the boundary conditions (3.18) and (3.19).

### 3.4 Galerkin discretization in space

Using the well established method of weighted residuals, the weak form of the governing equation (3.22) is obtained as

$$\int_0^l w(x)r(x, t) \, dx = 0 \quad (3.23)$$

where

$$w = \text{test function}, \quad w = \sum_{i=1}^{n_{eq}} N_i w_i \quad ; \quad N_i = \text{finite element basis function}.$$ 

The discretization in space in this work is performed with the classical piecewise linear nodal basis functions. Node $i = 1$ is at $x = 0$, node $i = n_{eq}$ is at the cold face, $x = \ell$.

Thus, we obtain

$$\int_0^l N_i r \, dx = 0, \quad i = 1, \ldots, n_{eq} \quad (3.24)$$

The term $\int_0^l w \frac{\partial}{\partial x} (k \frac{\partial T}{\partial x}) \, dx$ is treated (as is well established) with integration by parts, which brings in the natural boundary conditions

$$\int_0^l w \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) \, dx = - \int_0^l \frac{\partial w}{\partial x} k \frac{\partial T}{\partial x} \, dx + \left[ w k \frac{\partial T}{\partial x} \right]_0^l$$

$$= - \int_0^l \frac{\partial w}{\partial x} k \frac{\partial T}{\partial x} \, dx - \left[ w q \right]_0^l \quad i = 1, 2, \ldots, n_{eq} \quad (3.25)$$
Thus, the weak form may be written as

\[
\int_0^l N_i \rho c_p \frac{\partial T}{\partial t} \, dx + \int_0^l \frac{\partial N_i}{\partial x} k \frac{\partial T}{\partial x} \, dx + \int_0^l N_i \frac{\partial \rho}{\partial t} \left( c_p - c_{pg} \right) T \, dx + \int_0^l N_i \left( \int_0^x \frac{\partial \rho}{\partial t} \, dx \right) c_{pg} \frac{\partial T}{\partial x} \, dx \\
+ \int_0^l N_i Q \frac{\partial \rho}{\partial t} \, dx + [N_i q]_0^l = 0 \quad i = 1, 2, \ldots, n_{eq}
\]  

(3.26)

with the initial conditions \( \rho(0) = \rho_v, T(0) = T_i \). It needs to be realized that \( \rho \) and \( \frac{\partial \rho}{\partial t} \) depend nonlinearly on the temperature through (3.13). Furthermore, \( k \) and \( c_p \) are also nonlinear functions of \( T \) because they are expressed as the properties of the solid phase through the law of mixtures (3.11) and (3.12), and \( F \) is related to \( \rho \) through (3.15).

Representing the temperature trial function with the finite element expansion

\[
T(t, x) = \sum_{j=1}^{n_{eq}} N_j(x) T_j(t)
\]  

(3.27)

the first-order nonlinear matrix ordinary differential equation is obtained

\[
M \dot{\Theta} + \left( K_c + K_d + K_g + K_s \right) \Theta + L = 0
\]  

(3.28)

where

\begin{align*}
\Theta &= \text{ vector of temperatures} \\
M &= \text{ capacitance matrix} \\
K_c &= \text{ thermal conductivity matrix} \\
K_d &= \text{ decomposition matrix} \\
K_g &= \text{ gas convection matrix} \\
K_s &= \text{ surface heat transfer matrix} \\
L &= \text{ thermal load vector}
\end{align*}

All of the above matrices are nonlinear functions of \( T \). In what follows the notation \( \bar{K} = K_c + K_d + K_g + K_s \) shall be used. In components one has

\[
\Theta_i = T_i
\]  

(3.29)

\[
M_{ij} = \int_0^l N_i \rho c_p N_j \, dx
\]  

(3.30)
\[ K_{c,ij} = \int_{0}^{l} \frac{\partial N_i}{\partial x} k \frac{\partial N_j}{\partial x} dx \]  
(3.31)

\[ K_{d,ij} = \int_{0}^{l} N_i \frac{\partial \rho}{\partial t} (c_p - c_{pg}) N_j dx \]  
(3.32)

\[ K_{g,ij} = \int_{0}^{l} N_i \left( \int_{t}^{l} \frac{\partial \rho}{\partial t} dx \right) c_{pg} \frac{\partial N_j}{\partial x} dx \]  
(3.33)

\[ K_{s,11} = k_{s,hot}, \quad K_{s,n_{eq}n_{eq}} = k_{s,cold}, \quad \text{otherwise} \quad K_{s,ij} = 0 \]  
(3.34)

\[ L_1 = -h + \int_{0}^{l} N_i Q \frac{\partial \rho}{\partial t} dx + k_{s,hot} T_{fl} \]

\[ L_j = \int_{0}^{l} N_j Q \frac{\partial \rho}{\partial t} dx \quad j = 2, \ldots, n_{eq} - 1 \]  
(3.35)

\[ L_{n_{eq}} = -k_{s,cold} T_a . \]

The corresponding initial condition is \( \Theta_j(0) = T_{ini} \).

3.5 Time discretization

The classical Crank–Nicolson approximation (trapezoidal rule) is used

\[ \Theta_{m+1} = \Theta_m + \frac{\Delta t}{2} \left( \dot{\Theta}_{m+1} + \dot{\Theta}_m \right) , \]

where

\[ \Theta_j = \Theta(t_j) \]
\[ \dot{\Theta}_j = \dot{\Theta}(t_j) \]
\[ \Delta t = t_j - t_{j-1} . \]

Thus, one may express

\[ \dot{\Theta}_{m+1} = \frac{2}{\Delta t} \left( \Theta_{m+1} - \Theta_m \right) - \dot{\Theta}_m \]

and

\[ M_{m+1} \dot{\Theta}_{m+1} = \frac{2}{\Delta t} M_{m+1} \left( \Theta_{m+1} - \Theta_m \right) - M_{m+1} \dot{\Theta}_m , \]  
(3.36)
where
\[ M_{m+1} = M(\Theta_{m+1}). \]

Note that \( \dot{\Theta}_m \) may be expressed from
\[ M_m \dot{\Theta}_m + \bar{K}_m \Theta_m + L_m = 0 \quad \Rightarrow \quad \dot{\Theta}_m = M_m^{-1}(-\bar{K}_m \Theta_m - L_m) \quad (3.37) \]

Hence, the dynamic balance equation at \( t_{m+1} \) may be written as
\[ R(\Theta_{m+1}) = \left( \frac{2}{\Delta t} M_{m+1} + \bar{K}_{m+1} \right) \Theta_{m+1} - M_{m+1} \Theta_m - \frac{2}{\Delta t} M_{m+1} \Theta_m + L_{m+1} = 0. \quad (3.38) \]

Thus, the time stepping algorithm is obtained
\[ \begin{align*}
\Theta_0 &= \text{given} \\
\Theta_0 &= M_0^{-1} \left( -\bar{K}_0 \Theta_0 - L_0 \right) \\
j &\leftarrow 1 \\
\text{while} \text{ target time not reached} \\
\text{solve} \ R(\Theta_j) &= 0 \text{ for } \Theta_j \\
\dot{\Theta}_j &= M_j^{-1} \left( -\bar{K}_j \Theta_j - L_j \right) \\
j &\leftarrow j+1 \\
\text{done while}
\end{align*} \]

The solution of the nonlinear algebraic equations (3.38) may be obtained quite efficiently with a Newton’s solver: Using
\[ R \left( \Theta_{m+1}^{(k)} \right) = R \left( \Theta_{m+1}^{(k-1)} \right) + \frac{\partial R \left( \Theta_{m+1}^{(k-1)} \right)}{\partial \Theta_{m+1}} \Delta \Theta^{(k)} \approx 0 \quad (3.39) \]
we obtain the algorithm
\[ \begin{align*}
\Theta_{m+1}^{(0)} &= \Theta_m \\
k &\leftarrow 1 \\
\text{while} \text{ not converged} \\
\Theta_{m+1}^{(k)} &= \Theta_{m+1}^{(k-1)} + \Delta \Theta^{(k)} \text{, where} \\
\Delta \Theta^{(k)} &= - \frac{\partial R \left( \Theta_{m+1}^{(k-1)} \right)}{\partial \Theta_{m+1}} R \left( \Theta_{m+1}^{(k-1)} \right) \\
k &\leftarrow k+1 \\
\text{done while}
\end{align*} \]
The tangent $\partial R/\partial \Theta$ is approximated in this work as
\[
\frac{\partial R}{\partial \Theta_{m+1}} \approx \frac{2}{\Delta t} M_{m+1} + \dot{K}_{m+1}
\] (3.40)
that is $\partial M_{m+1}/\partial \Theta_{m+1}$, $\partial K_{m+1}/\partial \Theta_{m+1}$, $\partial L_{m+1}/\partial \Theta_{m+1}$ are all neglected. Despite this simplification, convergence is quite satisfactory. In fact, the average number of iterations needed in a representative example was about four, and the maximum number of iterations required at any time step was only five.

### 3.5.1 Update of the mass density of the solid phase

Notice that $\rho$ appears in the formulation as a constitutive variable. Thus, only its values (and the values of its derivatives) at the quadrature points are needed. Since they depend on $\Theta_{m+1}$, it is necessary to formulate an update algorithm. The update should be implicit so as not to destroy the stability of the scheme, which at least for the linear regime should be unconditionally stable.

A trapezoidal rule (Crank–Nicolson) is formulated for $\rho$, or equivalently for $F$ from the evolution equation (3.14). Thus, we use
\[
F_{m+1} = F_m + \frac{\Delta t}{2} \left( \frac{\partial F}{\partial t} \bigg|_m + \frac{\partial F}{\partial t} \bigg|_{m+1} \right)
\] (3.41)
from which $\frac{\partial F}{\partial t} \bigg|_{m+1}$ is expressed, and the update algorithm is obtained in the form of the equation
\[
\frac{2}{\Delta t} \left( F_{m+1} - F_m \right) - \frac{\partial F}{\partial t} \bigg|_m = A \left( \frac{\rho_v - \rho_{ch}}{\rho_v} \right)^{n-1} \exp \left( -\frac{E_a}{RT_{m+1}} \right) F^n_{m+1} = 0 \ , \ (3.42)
\]
that needs to be solved for $F_{m+1}$. If $n = 1$ (that is for a first-order reaction), the solution may be obtained explicitly as
\[
F_{m+1} = \frac{2 \Delta t F_m + \frac{\partial F}{\partial t} \bigg|_m}{2 \Delta t + A \exp \left( -\frac{E_a}{RT_{m+1}} \right)}
\] (3.43)
Otherwise, equation (3.42) may be solved with straightforward Newton iteration.

Recall that $F_0 = 1$, and the initial condition $T_0 = T_{ini}$ then supplies
\[
\frac{\partial F}{\partial t} \bigg|_0 = -A \left( \frac{\rho_v - \rho_{ch}}{\rho_{ch}} \right)^{n-1} \exp \left( -\frac{E_a}{RT_0} \right) F^n_0 \ . \ (3.44)
\]
The subsequent values $F_1, F_2, \ldots$ may be then obtained from the update formula as needed for the evaluation of the weak form.
3.6 Validation and experiments

3.6.1 Polyester-based glass reinforced panel

The data for this problem has been obtained from Looyeh et al. [59], who seems to have used as their source Wu et al. [91] for most of their material data and experimental measurements.

The structure is a single laminate plate of thickness 10.9 mm. The material is polyester resin (represented with subscript \(r\)) with glass fiber reinforcement (45% of the volume, represented with subscript \(f\)). The material properties are given in Reference [59] as:

\[
\begin{align*}
A & = 1.0 \times 10^3 \text{ [sec}^{-1}] ; \\
c_{pf} & = 760 \text{ (specific heat of the fiber material) [J kg}^{-1} \text{ K}^{-1}] \\
c_{pr} & = 1,600 \text{ (specific heat of the resin) [J kg}^{-1} \text{ K}^{-1}] \\
c_{pg} & = 2,386.5 \text{ (specific heat of the gas) [J kg}^{-1} \text{ K}^{-1}] \\
E_a & = 0.5 \times 10^5 \text{ [kJ kg}^{-1} \text{ mole}^{-1}] \\
k_f & = 1.04 \text{ (thermal conductivity of the fiber material) [W m}^{-1} \text{ K}^{-1}] \\
k_r & = 0.20 \text{ (thermal conductivity of the resin) [W m}^{-1} \text{ K}^{-1}] \\
Q & = -2.3446 \times 10^5 \text{ [J kg}^{-1}] \\
V_f & = 0.45 \text{ (volume fraction of the fibers) [ND]} \\
\rho_v & = 1812.0 \text{ (mass density of the composite) [kg m}^{-3}] \\
\rho_f & = 2560.0 \text{ (mass density of the fiber material) [kg m}^{-3}] \\
\rho_r & = 1200.0 \text{ (mass density of the resin) [kg m}^{-3}] \\
n & = 1 \text{ (order of the reaction) [ND]}
\end{align*}
\]

Note that none of these material parameters depend on temperature. The ambient temperature \(T_a\) is assumed to be constant at 293 K, which is also the initial temperature of the plate, \(T_{ini}\). The cold face is assumed to be insulated (zero heat flux, \(k_{s,cold} = 1\)), the hot face is loaded with a heat insult in the form of prescribed temperature. Thus, the hot face boundary condition reads

\[
q(t, 0) = -k_{s,hot} [T(t, 0) - T_f(t)]
\] (3.45)
where
\[ k_{s,hot} = 5 \times 10^6 \text{ (penalty parameter) [W m}^{-2}\text{ K}^{-1}] \]
\[ T_{fl} = T_a + (1273 - T_a) (1 - \exp [-\exp (0.71 \log(t/124.8))]) \text{ [K]} \]

**Thermal conductivities of the virgin material and charred residue**

The thermal conductivities of the virgin material and of the residue of the decomposition of the composite (char) are not available from Reference [59]. Therefore, these two quantities have been estimated from the following formulas. Clearly, experimentally determined quantities will be superior to these estimates, especially if determined as a function of temperature.

The thermal conductivity of the virgin laminate was estimated using a relationship developed by Reference [83] (see also Reference [10]) for a heterogeneous medium with cylindrical inclusions (fibers) at volume fraction \( V_f \), in the direction perpendicular to the fibers:

\[
\frac{k_v}{k_r} = 1 + \frac{2V_f}{k_r + k_f} - V_f + \left( \frac{k_r - k_f}{k_r + k_f} \right) (0.3058V_f^4 + \ldots) \tag{3.46}
\]

where
\[ k_r = \text{ thermal conductivity of the resin [W m}^{-1}\text{ K}^{-1}] ; \]
\[ k_f = \text{ thermal conductivity of the fiber material [W m}^{-1}\text{ K}^{-1}] . \]

For this particular resin, the thermal conductivity of the char may be roughly estimated by viewing the residue of decomposition as mainly fibers with voids where the resin used to be. A model has been developed by Reference [44] (see also References [55, 10]) for a solid with parallel planar fissures (gas pockets) perpendicular to the direction of heat flow:

\[
\frac{k_{ch}}{k_f} = \frac{1}{1 - V_f + \left( \frac{k_{air}}{k_fV_f + \frac{4\sigma T^3 L}{k_f}} \right)^{-1}} \tag{3.47}
\]
Figure 3.2: Convergence of the temperature as a function of the spatial resolution (number of elements). Note that the 10, 20, 40 and 80 element discretizations are virtually indistinguishable in the plot. The markers represent the corresponding experimental data.

where

\[ k_{\text{air}} = \text{thermal conductivity of the air [W m}^{-1} \text{K}^{-1}] \],
\[ \sigma = \text{Stefan-Boltzmann constant, } \sigma = 5.67 \times 10^{-8} \text{ [W m}^{-2} \text{K}^{-4}] \],
\[ L = \text{total thickness of the material in the direction of heat conduction [m]} \].

This formula has been utilised with \( T \approx T_{\text{avg}} = 400 \text{ K} \).

**Convergence of the space discretization**

As the mesh is refined, and as the time step is decreased, convergence in both cases is achieved. Figure 3.2 shows the convergence of the simulation as the spatial discretization is refined. As the number of elements (10, 20, 40, and 80 elements) is increased with the time step held constant, it is clear that convergence is achieved since all results fall essentially on a visually indistinguishable curve.

**Convergence of the time discretization**

Figure 3.3 shows the convergence as the time step is reduced. Here a ten element model is used, and the time step is defined as a multiple of the critical time step for the ten element case (\( \Delta t_{\text{crit}} = 9.34 \text{ s} \)). (The critical time step \( \Delta t_{\text{crit}} \) is the stability...
Figure 3.3: Convergence of the temperature as a function of the time step length.

Figure 3.4: Evolution of the mass density for a 20-element mesh.

limit for the forward Euler discretization of the corresponding linearization at $t = 0$.) Figure 3.3 shows results for time step of 8, 2, 0.5, and 0.125 times the critical time step, and again convergence occurs fairly rapidly.

3.7 Conclusions

A robust and consistent finite element model of the coupled nonlinear partial differential equations provided by Henderson, Wiebelt, and Tant [37] has been formulated to describe the behavior of fiber reinforced polymer composites during exposure to a thermal load (fire). The evolving mass density is treated as a constitutive variable, and is updated with a fully implicit algorithm. In combination with the overall implicit time stepping (Crank–Nicolson), a well-behaved and
quickly converging algorithm is obtained.

This finite element model has been used to predict the temperature distribution in a laminate plate made of polyester resin with glass fiber reinforcement [59]. Some material properties needed in our model were not available from experiment and had to be estimated. Moreover, the temperature dependence of the material properties, such as thermal conductivities and specific heats, were not available and had to be ignored. Under these constraints, the fit of experimental measurements of the temperature in time by the model is quite satisfactory.

To further increase the predictive capabilities of the present model, some presently ignored phenomena should be included: lack of thermal equilibrium between product gases and solid, accumulation of decomposition gases with attendant pressurization and volumetric expansion of solid, etc. Expansion of the model into two or three dimensions would be helpful for structures of complex geometry. Also, clearly an adaptive framework would be helpful, especially in the time direction.

\section{3.8 Acknowledgements}

Chapter 4

Thermal model material properties

4.1 Introduction

In this section accurate material properties for use in the thermal model developed in Chapter 3 are determined. This requires the definition of twenty input parameters that will describe the material response. These include ten parameters that describe the thermophysical behavior of the various materials, three that describe the degradation reaction, and three that describe the mass densities and heat of decomposition. As well, four boundary condition parameters need to be specified, in particular the convective heat transfer coefficient and the surface emissivity at both the hot and cold faces.

4.2 Thermophysical properties

Several thermophysical properties are required as input for the model. Thermophysical properties generally include thermal conductivity, specific heat, thermal diffusivity, etc. The present model requires that the thermal conductivity of the virgin composite ($k_v$) and char ($k_{ch}$) be defined, as well as the specific heat (at constant pressure) of the virgin composite ($c_{pv}$), char ($c_{pch}$), and product gases.
These thermophysical properties are commonly highly temperature-dependent. As such, the model is numerically implemented so as to allow each of these five properties to be inputted as an arbitrary mathematical function (in particular, as a function handle in MATLAB).

For practical purposes, and in order to simplify statistical analyses to be described in Chapter 5, these functions are defined via the following relations:

\[
\begin{align*}
    c_{pch} &= c_{pchm}(T - T_0) + c_{pchb} \\
    c_{pg} &= c_{pgm} \left( \log_{10}(T) - \log_{10}(T_0) \right) + c_{pgb} \\
    c_{pv} &= c_{pvem}(T - T_0) + c_{pveb} \\
    k_{ch} &= k_{chm}(T - T_0) + k_{chb} \\
    k_{v} &= k_{vem}(T - T_0) + k_{veb}
\end{align*}
\]

Thus we have ten input parameters which need to be defined—five slope values and five intercept values. Note that the intercept values are not necessarily the values at \( T = 0 \) K. In fact, the temperature at which intercept values are defined \( T_0 \) is simply a constant which must be specified. This flexibility aids in the statistical analyses to be described in Chapter 5.

Values for parameters relating to the specific heat of the char and virgin composite, and relating to the thermal conductivities of the char and virgin composite, are available from research conducted by Dr. Brian Lattimer at Hughes Associates, Inc. [50]. In particular, specific heat capacity values are obtained via data provided in Figure 4.1, and thermal conductivity values are obtained via data provided in Figure 4.2. These values have been measured for a specific e-glass/vinylester composite that is particularly relevant to the ONR, which is funding this research. In particular, it is a Saint-Gobain/Vetrotex 0.81 kg/m² E-glass woven roving and Derakane 510A brominated vinylester resin composite. It was fabricated via the SCRIAMPTM vacuum infusion process, to yield a composite with 30% resin by weight.

The data shown in Figures 4.1 and 4.2 provide slope and intercept values with \( T_0 \) taken to be 0°C, or 273.15 K. However, for the statistical analyses described
Figure 4.1: Specific heat capacity (constant pressure) of char and virgin composite (E-glass/vinylester) as function of temperature.

in Chapter 5, $T_0$ is selected to be 700 K. In particular, those analyses require each input parameter to be subjected to small perturbations. It is therefore desirable to set up the model such that these small perturbations in input parameter values do not disproportionately change the resulting material properties. Setting the intercept value at 700 K, which is roughly the average temperature in relevant simulations, helps to prevent the occurrence of negative values and large variations in the thermophysical constants as the input parameter values are perturbed. These would be more likely to occur were the perturbations in the slope value to pivot the property value line about an extreme temperature value.

Thus the slope values are identical to those provided in the figures, while the intercept values are obtained by evaluating the expressions provided to determine the parameter value at $T = 700 \text{ K} - 273.15$, with this value adjusted to account for the fact that the experimental values are in degrees Celsius.
Figure 4.2: Thermal conductivity of char and virgin composite (E-glass/vinylester) as function of temperature.

This process results in the following values:

\[
\begin{align*}
    c_{pch} &= 0.259 (T - 700) + 1151.6 \\
    c_{pv} &= 0.0452 (T - 700) + 1099.3 \\
    k_{ch} &= 2.83 \times 10^{-4} (T - 700) + 0.2157 \\
    k_{v} &= 4.404 \times 10^{-5} (T - 700) + 0.3308
\end{align*}
\]  

(4.2)

Here the temperature is provided in Kelvin, the resulting specific heat values are in J/(kg·K), and the resulting thermal conductivity values are in W/(m·K).

### 4.2.1 Specific heat of pyrolysis gases

Determination of the specific heat of the pyrolysis gases is more complex. This property was not measured directly by Dr. Lattimer for this material. Various values are available from the literature, however. Henderson et al. [37] used a constant value of 9630 J/(kg·K) which approximates temperature-dependent values given by Pittman and Brewer [68]. This value was apparently obtained for a
pyrolyzing nylon/phenolic sample—as such, it is not necessarily of value to the current application (i.e. e-glass vinylester). Looyeh et al. [59] first use a value of 2386.5 J/(kg · K), which is attributed to a “number of sources” with only a technical report by Wu et al. [91] explicitly noted. In later papers the temperature-dependent relation 2386.5 + 1.05T is used, where the temperature is provided in degrees Celsius and the resulting specific heat is in J/(kg·K) [58], and the previous paper (not containing the temperature-dependent relation) is cited as the source. However, these material properties are intended to represent a e-glass polyester composite, so their validity in the current application is doubtful for this reason as well.

In light of this lack of accurate data, an attempt was made to calculate the specific heat of the product gases in two steps—first, the product gases would be determined; and second, the temperature-dependent properties of the individual gases would be combined to obtain a reasonable estimate for the properties of the mixture. The specific product gases produced during the pyrolysis of e-glass vinylester composite may be determined by gas chromatography/mass spectrometry. For a complete discussion of this technique, and the determination of composition quantities from spectrographs, see Kitson et al. [48]. Specific composition data are available in some form from a number of sources (a comprehensive review is provided by Haken [32]). Cunliffe et al. [17] provide data for the product gases of glass vinylester composite; however they are only provided as a cumulative total, and no estimate of the change in composition with increasing temperature is provided. Hiltz [40] likewise provides a chromatogram for a vinylester resin sample (Derakane 510A40). However, this chromatogram, which could be used to determine relative concentrations of the component gases, is only provided at a temperature of 800°C. Regnier, however, does provide thermally-dependent composition data for the pyrolysis gases produced by a burning glass vinylester composite [70]. The resin is in particular Derakane D411 with a 45% styrene by weight ratio. However, these data are provided only at 200°C, 400°C, 480°C, and 600°C. Of the gases specified, thermally-dependent specific heat data are available for three: styrene, phenyl propane (120 molar mass—aka cumene), and toluene [90]. The proportions
Table 4.1: Composition of pyrolysis gases with temperature

<table>
<thead>
<tr>
<th></th>
<th>200°C</th>
<th>400°C</th>
<th>480°C</th>
<th>600°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Styrene</td>
<td>14.8%</td>
<td>59.5%</td>
<td>81.5%</td>
<td>92.0%</td>
</tr>
<tr>
<td>Cumene</td>
<td>13.7%</td>
<td>2.5%</td>
<td>1.3%</td>
<td>0.5%</td>
</tr>
<tr>
<td>Toluene</td>
<td>0.0%</td>
<td>0.0%</td>
<td>0.0%</td>
<td>4.9%</td>
</tr>
<tr>
<td>Total</td>
<td>28.5%</td>
<td>62.0%</td>
<td>82.8%</td>
<td>97.4%</td>
</tr>
</tbody>
</table>

of these product gases as a function of temperature are provided in Table 4.1. As will be shown in Section 4.3, pyrolysis begins at around 300°C–350°C, and ends at around 375°C–425°C; the position within this range is determined by the heating rate. Clearly within this range, roughly half of the gases produced are accounted for. While this is less than desired, it may produce a reasonable estimate. Per Reid et al., the specific heat of the mixture may be obtained via the component gas properties according to the relation

\[ c_{pg,m} = \sum_i y_i c_{pg,i} \]  

where \( y_i \) is the mole (or volume) fraction of component \( i \). Note that this is true for ideal gases—in the current application this will be approximately true. Via interpolation, the product gases at various temperatures can be estimated (using the limiting values at the 200°C and 600°C limits for values below and above them, respectively). The product gas specific heats may then be interpolated at those temperatures (via the data from Touloukian et al. [90]), and combined via Equation (4.3). The resulting values are plotted in Figure 4.3. Figure 4.3 also shows other values provided in the literature (as previously mentioned), and how they compare to the values predicted via the current method—indeed the comparison is reasonable. In fact the mixture is seen to closely track the behavior of styrene, as styrene forms a majority of the product gases. The data provided by Hiltz confirms that styrene makes up a majority of the gases produced at a temperature of 800°C [40]. A regression of the data resulting from this model yields the expression

\[ c_{pg} = 2546 (\log_{10}(T) - \log_{10}(700)) + 2246 \]  

(4.4)
where again the temperature is provided in Kelvin and the resulting specific heat value is in J/(kg·K). This expression is formulated so that it results in a linear relationship on a log-linear plot, as this is the behavior observed in Figure 4.3. To perform a linear regression on this data, one first takes the logarithm of all temperature values, and then one performs a linear regression on the resulting values and the corresponding specific heat values.

### 4.3 Arrhenius reaction constants

The pyrolytic decomposition of the E-glass/vinylester composite material is modelled using an Arrhenius reaction equation of arbitrary order, namely

\[
\frac{\partial \rho}{\partial t} = -A\rho_v \left( \frac{\rho - \rho_{ch}}{\rho_v} \right)^n \exp \left( -\frac{E_a}{RT} \right).
\]  

(4.5)

Thus the pre-exponential constant \( A \), the activation energy \( E_a \), and the reaction order \( n \) must be determined. These data are commonly determined via plots of mass vs. temperature at multiple heating rates obtained via thermogravimetric
analysis (TGA), as discussed in Section 1.4.3. Such data is available via Lattimer and Ouellette for the material of interest, and is provided in Figure 4.4. These data were obtained for the E-glass/vinylester composite material of interest ground into a powder. This is desirable as one aims to make the surface area of the sample as large as possible for TGA analysis, such that the decomposition behavior is not delayed by heat transfer effects, etc., as the delays resulting from heat transfer effects are accounted for elsewhere in the thermal model. Furthermore, the data was obtained via analysis in an inert (100% nitrogen) environment. This is necessary to duplicate the in situ decomposition behavior, as in a backward-smoldering environment the resin decomposes in the presence of inert pyrolysis gases, and in the absence of oxygen.

The activation energy may be obtained via such TGA data using various methods, for instance the Flynn and Wall method [24], the Coats and Redfern method [15], and Friedman’s multiple heating rate technique [25]. As an example, such thermogravimetric data for the decomposition of vinylester resin alone is

Figure 4.4: Thermogravimetric analysis results for powder sample

![](image.png)
available from Gaur and Rai [27]. This reference provides data for use with both the Flynn and Wall [24], and the Coats and Redfern [15] methods.

For the commonly used Flynn and Wall method, thermogravimetric analysis is performed at multiple heating rates. The quantity $-\log_{10}(\beta)$, where $\beta$ is the heating rate, is then plotted vs. the reciprocal of the absolute temperature for various degrees of conversion. This data is plotted in Figure 4.5 for the current material of interest. $E_a$ values are obtained from the slopes of regression lines at each constant degree of conversion. An average $E_a$ value is then calculated from the mean of these values. The resulting average $E_a$ value obtained via the plotted data is $1.6758 \times 10^5$ J/mol.

Thus one of the three Arrhenius reaction constants is known, and the other two must still be determined. For this purpose a two parameter optimization was performed. This involved solving the differential equation (Equation (4.5)) for all five heating rates, taking the norm (largest singular value) of the difference between the experimental and model data (interpolated at temperatures ranging

![Figure 4.5: Determination of activation energy via Flynn and Wall technique](image)

Figure 4.5: Determination of activation energy via Flynn and Wall technique
from 50°C to 447°C), and then minimizing this “score.”

The differential equation (Equation (4.5)) was solved via the `ode15s` MATLAB function—other MATLAB solvers could not operate across the full spectrum of Arrhenius reaction parameter values. The absolute and relative error tolerances for use by this function were set to 0.01, and these errors were specified to be controlled relative to the norm of the solution.

The two-parameter optimization took the form of performing one-parameter optimizations (via the `fminbnd` MATLAB function) to find \( A \) for specified ranges of values for \( n \). The “score” was then plotted over the \( n \) values—the minimum in this case was clearly visible. The range for \( n \) was then refined, and the process completed, until the \( n \) value was determined to three significant figures.

The resulting value for \( A \) is \( 2.18 \times 10^{11} \) Hz, corresponding to a value for \( n \) of 1.14. The optimal fit is shown in Figure 4.6.

![Optimal fit to TGA data](image)

Figure 4.6: Optimal fit to TGA data
4.3.1 Mass densities and heat of decomposition

The mass densities of virgin composite and char for the E-glass/vinylester composite of interest are given by Lattimer and Ouellette as $\rho_v = 1683 \text{ kg/m}^2$, and $\rho_{ch} = 1235 \text{ kg/m}^2$ [50].

The heat of decomposition for this material is also provided by Lattimer and Ouellette [50]. They provide a value that was obtained via a thermal decomposition apparatus, in which a small sample is exposed to a known heat flux. With this apparatus a ramping heat flux test was performed. The heat of decomposition was determined via predicting the decomposition behavior with a model which neglects the convection of the pyrolysis gases, and then varying the heat of decomposition value to minimize the least squares difference between the measured and predicted sample mass. This results in a value of $-800 \text{ kJ/kg}$, where the negative sign indicates that the reaction is endothermic (test performed in an inert, 100% nitrogen environment). However, the effect of the pyrolysis gases is expected to be significant (as discussed in Chapter 5), thus this value should be treated with caution.

Lattimer and Ouellette also measure the heat of decomposition of this composite via differential scanning calorimetry (DSC, discussed in Section 1.4.3) for samples in coupon, powder, and fragment form. The resulting heat of decomposition values are $-800$, $-595$, and $-602 \text{ kJ/kg}$, respectively. For the current purpose the value for powder is preferred, as this value will have maximum surface area, and thus will be free to fully react, unimpeded by heat transfer effects. Thus the heat of decomposition is taken to be $-5.95 \times 10^5 \text{ J/kg}$.

4.3.2 Boundary condition parameters

The thermal boundary condition used to represent the fire may vary. It will generally either take the form of a defined temperature curve or a defined heat flux. These are then applied at the panel boundary using relations for convective and radiative heat transfer. In particular, the thermal boundary condition at the
hot face may take the form

\[ q'' = \epsilon_h \dot{q}'' + k_{sh} (T_{fl}(t) - T(t, 0)) + \epsilon_h \sigma \left( (T_{fl}(t))^4 - (T(t, 0))^4 \right), \]  

(4.6)

and at the cold face

\[ q'' = k_{sc} (T(t, t) - T_a(t)) + \epsilon_c \sigma \left( (T(t, t))^4 - (T_a(t))^4 \right). \]  

(4.7)

In this the heat flux, \( q'' \), is a function of surface emissivities \( \epsilon \), convection heat transfer coefficients \( k_s \), a prescribed heat flux at the hot face \( q'' \), a prescribed flame temperature \( T_{fl}(t) \), an ambient temperature at the cold face \( T_a \), and the Stefan–Boltzmann constant, \( \sigma = 5.670 \times 10^{-8} \text{ J/(K}^4 \cdot \text{m}^2 \cdot \text{s}) \).

Models have typically been run using values for surface emissivity of 0.85 for the composite and 0.45 for Structo-Guard insulation (commonly used to protect these panels during tests). The value typically used for the convection heat transfer coefficient in an experimental furnace is \( k_{sh} = 13 \text{ W/(m}^2 \cdot \text{K}) \); while at the cold face, a value of \( k_{sc} = 10 \text{ W/(m}^2 \cdot \text{K}) \) has been assumed. The surface emissivities and the furnace convection heat transfer coefficient were provided via personal correspondence by Dr. Brian Lattimer at Hughes Associates. Typical convection heat transfer coefficient values for free convection range from 5–25 W/(m\(^2\)·K) [42].

A few relevant temperature curves that are commonly used in these simulations include the curve given by ASTM standard E 119–00a for building materials, specified in Table 4.2 [9]; the UL 1709 temperature curve (intended to represent a petroleum pool fire), included in Table 4.3; and the IMO/FTP temperature curve for commercial ships, defined by the function \( T = 345 \log_{10}(8t + 1) + 20 \), where \( t \) is the time in minutes, and \( T \) the resulting temperature in degrees Celsius.

### 4.4 Conclusions

Twenty thermal property parameters must be specified to accurately run this model. In this chapter, these parameters have been determined for a material of particular interest to this research.

Of these twenty parameters, there is significant uncertainty in the values specified for the specific heat of the pyrolysis gases, due to the fact that all of the
Table 4.2: ASTM E 119–00a Time/Temperature Curve (these points determine the character of the curve—however, the curve is not linear between these points. In practice, the interpolation is performed using piecewise cubic Hermite interpolation (i.e. the cubic option in \texttt{interp1} MATLAB function.)

<table>
<thead>
<tr>
<th>Time</th>
<th>Temp. (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>20°C</td>
</tr>
<tr>
<td>5 min</td>
<td>538°C</td>
</tr>
<tr>
<td>10 min</td>
<td>704°C</td>
</tr>
<tr>
<td>30 min</td>
<td>843°C</td>
</tr>
<tr>
<td>1 h</td>
<td>927°C</td>
</tr>
<tr>
<td>2 h</td>
<td>1010°C</td>
</tr>
<tr>
<td>4 h</td>
<td>1093°C</td>
</tr>
<tr>
<td>8 h</td>
<td>1250°C</td>
</tr>
<tr>
<td>∞</td>
<td>1250°C</td>
</tr>
</tbody>
</table>

Table 4.3: UL 1709 Time/Temperature Curve.

<table>
<thead>
<tr>
<th>Time</th>
<th>Temp. (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>27°C</td>
</tr>
<tr>
<td>5 min</td>
<td>1092°C</td>
</tr>
<tr>
<td>∞</td>
<td>1092°C</td>
</tr>
</tbody>
</table>
product gases were not accounted for in calculating this parameter. There is also significant uncertainty in the assumed value for the convection heat transfer coefficient at the cold face. These uncertainties will be quantified more precisely in the next chapter.
Chapter 5

Statistical characterization of thermal model

5.1 Introduction

In this chapter, sensitivity and uncertainty analyses are performed on the thermal model described in Chapter 3, and the results are reported. This effort quantitatively describes the model behavior, in terms of three things. First, it provides the relative magnitude of the impact that each input parameter has on the thermal prediction. This allows the input parameters to be sorted in terms of their relative importance to the temperature prediction. Input parameters which have a large affect on the predicted temperatures may then be more accurately determined; less effort should be expended in the accurate determination of those parameters which have negligible effect on the model output. Secondly, it describes quantitatively how the individual input parameter values affect the predicted temperatures. This allows one to form an educated opinion as to why a predicted result may be different from an experimental result, in terms of which input parameter values may be responsible for the discrepancy. Finally, this process allows for the predicted uncertainty of the model, due to the estimated uncertainty in the input parameters, to be quantified. This gives users of the model the ability to better understand the limitations upon the accuracy of the predicted temperature values due to un-
certainty with the input parameter values. This does not characterize uncertainty due to the inability of the model to fully represent the chemistry or physics of the problem. The results from this statistical characterization of the model are then used to validate it with respect to experimental data available from the literature.

The broad goal of this work is to understand the behavior of an E-glass vinylester composite structure when exposed to fire in a marine application. However, for design purposes, the likely response of such a structure in this situation is not enough—some characterization of the uncertainty in that response should be provided, such that design criteria containing a sufficient factor of safety may be specified.

The structural behavior of such a structure when exposed to fire may be determined via a coupling of several models; including a thermal model, a model of mechanical property degradation with temperature, and a material model encapsulating this degraded behavior implemented into a finite element structural model. To characterize the variability in this behavior, therefore, an uncertainty analysis of all of these coupled models should be performed. To determine how this prediction responds to changes in the input parameters, a sensitivity analysis of the coupled models should be performed. This effort is a step in that direction, such a characterization of the first of these models.

The plan of this chapter is as follows: first, local methods of sensitivity analysis will be discussed, and one such method will be applied to the model. The results will be presented and interpreted. Second, a Monte Carlo analysis will be performed on the model, using Latin hypercube sampling. A lack of experimental characterization of input parameter uncertainty precludes a definitive simulation at this point. Regardless, an exploratory analysis will be performed using hypothesized input parameter distributions. A Monte Carlo based uncertainty analysis will then be performed on the model and the uncertainty in the predicted thermal output characterized. Third, techniques of global sensitivity analysis will be described, and the results of such an analysis performed with the Monte Carlo simulation data will be presented. Finally, the results of these analyses will be used to validate the model with respect to experimental data available from the
5.2 Thermal model

The thermal model was described in detail in Chapter 3. The twenty input parameters which are utilized by the model have been defined and experimental values specified in Chapter 4. In this section, these twenty input parameters will be listed again for ease of reference.

The thermal model described in Chapter 3 requires the definition of twenty input parameters. These include ten parameters which define the behavior of the thermophysical constants—five of which are slope values, and five of which are intercept values. In particular, $c_{p,chb}$ and $c_{p,chn}$, which define the temperature dependent behavior of the specific heat at constant volume of the char; $c_{pgb}$ and $c_{pgm}$, which define the behavior of the specific heat of the product gases; and $c_{pvb}$ and $c_{pvm}$, which define the behavior of the specific heat of the virgin composite; are required. Also included in these are $k_{chb}$ and $k_{chn}$, which define the temperature dependent thermal conductivity of the char; and $k_{vb}$ and $k_{vm}$, which define the thermal conductivity of the virgin composite. These parameters are defined more specifically in Equation (4.1), in which $T_0 = 700$ K.

Three input parameters must also be defined to describe the pyrolytic decomposition behavior of the composite. They are the Arrhenius reaction constants; namely a pre-exponential constant $A$, an activation energy $E_a$, and a reaction order $n$, as defined in Equation (4.5). The mass density of the char, $\rho_{ch}$, and of the virgin composite, $\rho_v$, must be defined. The heat of decomposition of the composite, $Q$, is also required.

Finally, four input parameters which describe the thermal behavior at the boundaries must be specified. These include the convection heat transfer coefficients at the hot and cold faces, $k_{sh}$ and $k_{sc}$, in addition to the surface emissivities of the hot and cold faces, $\epsilon_h$ and $\epsilon_c$, as employed for instance in Equations (4.6) and (4.7).
5.3 Methods of sensitivity analysis

Per Saltelli [71], sensitivity analysis (SA) methods may be grouped into screening methods, local SA methods, and global SA methods. Screening methods rank input parameters in order of importance, but do not yield information as to quantitatively how much more important one variable is than another. They typically are less computationally demanding than other methods, and thus are useful for more complex problems. The current model does not reach this level of complexity, and as such, more sophisticated SA techniques are preferable; therefore screening methods will not be discussed further.

Local SA techniques reveal the local effect of the input parameters on the model output. Local SA involves partial derivatives, which may be computed numerically by varying each input parameter within a small interval around a nominal value. Thus local SA methods vary one input parameter at a time, while holding others constant. This small interval is usually the same for all of the factors, and is therefore not related to the degree of knowledge of the input parameters.

Global SA, on the other hand, focuses on the global effect of the input parameters on the model output. It attempts to apportion the output variable uncertainty to the individual input parameters. Global SA varies all input parameters simultaneously, and varies each throughout the entire range of the expected variability in the input parameter. Statistical distributions for each input parameter are defined in the analysis, thus accounting for varying degrees of knowledge of the input parameters.

One problem with local SA methods is that one cannot accurately determine how the size of the variation of the input affects the output, unless the model is linear (the model described herein is not). Also, as parameters are varied one at a time, these methods cannot capture complex interactions between parameters as they change simultaneously. In general, if the input parameter uncertainty is large, local sensitivities alone don’t provide a reliable estimator of the output uncertainty in the model. Per Campolongo et al., a global SA should be performed if the model is nonlinear and various input parameters are affected by uncertainties of different orders of magnitude [71].
The current model is known to be nonlinear. Although the input parameter uncertainties have not been definitively characterized, it is hypothesized that different input parameters have significantly different uncertainties. As such, the reliability of any local analysis may not be great. However, the input parameter statistical distributions on which the global SA will be based are only approximated, detracting from the accuracy of the global SA. The current work will therefore provide results for both local SA and global SA of the model. The results will then be compared, and if they are found to agree, they may be viewed with greater confidence.

5.4 Local sensitivity analysis

The model presented in Chapter 3 may be represented as a function of the form

\[ y = f(x, t) \]  

(5.1)

where \( y \) is a vector of the time dependent model outputs (temperature, or alternatively mass density values) and \( x \) is a vector of the twenty model input parameters (thermophysical constants, reaction constants, etc.). The input parameter values may be perturbed, i.e. the input parameter values may be varied by a small amount. A first order Taylor series approximation of \( y \) may then be developed,

\[ y(x + \Delta x, t) \approx y(x, t) + \sum_{j=1}^{n} \left[ \frac{\partial y}{\partial x_j} \right] (\Delta x_j) \]  

(5.2)

Here the partial derivatives \( \frac{\partial y}{\partial x_j} \) are called first order local sensitivities, and \( n \) is the number of input parameters.

Two methods of determining the first order local sensitivities are indirect methods and direct methods. Indirect methods, or brute force methods, evaluate these partial derivatives numerically using finite-difference approximations such as

\[ \frac{\partial y}{\partial x_j} \approx \frac{y(x_j + \Delta x_j) - y(x_j)}{\Delta x_j}, \quad j = 1, \ldots, n. \]  

(5.3)

Per [71], the parameter change should not be too large (e.g. > 5%), so as not to damage the assumption of local linearity. It should also not be so small that
round-off error becomes significant. An acceptable value should be found by trial-and-error, beginning with say a 1% perturbation.

Direct methods for obtaining the first order local sensitivities, on the other hand, take a differential equation form of (5.1), and differentiate using the chain rule. This yields an ordinary differential equation solution for the sensitivity coefficients to be solved alongside the original model. However, this method requires the calculation of the Jacobian matrix. Our solution of the model uses an approximation of the Jacobian. As the exact Jacobian is not readily available, solving for the sensitivity coefficients using a direct method is deemed inexpedient, and it therefore is not pursued further.

To compare the effects of the various input parameters on the output variables, the first order local sensitivities may be normalized, for instance as follows,

\[
\frac{\partial y}{\partial x_j} \frac{x_j}{y}.
\]  

(5.4)

The coefficients may then be directly compared between variables.

For the purposes of this analysis, the model was run for a single panel of thickness 12.66 mm, to match the sample tested by Lattimer and Ouellette [50]. The input parameter values used were those provided in Chapter 4, except for the boundary condition parameters, which were as follows: \( \epsilon_c = 0.02, \epsilon_h = 0.94, k_{sc} = 1 \text{ W/(m}^2\cdot\text{K)} \), and \( k_{sh} = 7 \text{ W/(m}^2\cdot\text{K)} \). These values were used to duplicate the experimental results given in that paper. All values were varied by 1.0% according to Equation (5.3). Note that changing this percentage did not appear to have a significant effect on the results.

The values for the normalized first order local sensitivities thus obtained for these input parameter values and the resulting thermal output are shown in Figure 5.1. The y-axis of the bar chart is the normalized sensitivity coefficient value. Positive values indicate that increasing the input parameter value leads to an increase in the output variable value, and negative values indicate the opposite. For each input parameter, values throughout the simulation are shown, from the beginning of the simulation (left hand side) to the end of the simulation (right hand side). Thus the color change indicates the progression through time.
Figure 5.1: Normalized first order local sensitivity coefficients, indirect method. The input parameters are listed, the output variable is midpoint (top) and cold face (bottom) temperature. The values throughout the evolution of the problem are displayed for each input parameter, the varying shade from left to right indicates the time progression.
Figure 5.2: Normalized first order local sensitivity coefficients, indirect method. The input parameters are listed, the output variable is near-cold face mass density. The values throughout the evolution of the problem are displayed for each input parameter, the varying shade from left to right indicates the time progression.

The normalized first order local sensitivities taking the mass density as the output variable are provided in Figure 5.2. This shows that the coefficient for the mass density of the virgin material at the beginning of the simulation, and for the mass density of the char at the end of the simulation, are both equal to unity—as is to be expected.

The rank order of the absolute values of the normalized first order local sensitivity coefficients is shown in Figure 5.3. This figure provides insight into which of the various input parameters in the model are the most significant in terms of their impact on the predicted temperature at the given times. Figure 5.1 on the other hand demonstrates the effect that the input parameters have on the temperature at these locations throughout time. The results of this analysis will be discussed subsequently in conjunction with the results from the global analyses.

5.5 Monte Carlo analysis

A Monte Carlo analysis was performed on the model. Such an analysis involves assigning statistical distributions to each input parameter. These input parameter distributions are then sampled, and any expected correlations between the input
Figure 5.3: Rank order of absolute value of normalized first order local sensitivity coefficients with time. The input parameters are listed, the output variable is midpoint temperature (top) and cold face temperature (bottom). The higher the position in the figure, the more significant the parameter.
parameters are enforced upon the samples. These samples are then run through the given model, yielding corresponding output data. The resulting sampled input and corresponding output data may then be used in both an uncertainty analysis of the model output as well as in a global sensitivity analysis.

Limited experimental input parameter data are currently available, precluding full statistical characterization of each input parameter, along with correlations between them, at this time. However, it has been found that even a crude characterization of the input parameters may be adequate if the analysis is exploratory in nature [71]. For these purposes, distributions may be assigned over ranges of plausible values. Such assumptions will not generally have a great effect on the global sensitivity coefficients, though they can affect the uncertainty distributions of the output variables. With this in mind, a set of estimated input parameter probability distribution functions and correlations have been determined.

5.5.1 Input parameter statistical characterization

In general, normal distributions were used when data were unrestricted in range. Gamma distributions were used when data were restricted to all positive values. Triangular distributions were used when data were restricted with distinct nonzero lower and/or upper bounds.

Thermophysical constants

A normal distribution was used for all thermophysical constant slope and intercept values. Clearly slope values can be negative. Intercept values for specific heat may theoretically be negative. Even for the intercept values for thermal conductivity a normal distribution is used, though negative values are undesirable with the intercept defined at 700 K.

The slope and intercept values were determined via trial and error—in particular, the mean values are those provided in Chapter 4, while standard deviation values are estimated. The resulting distributions are sampled, and the samples are then plotted. This process is continued until the plotted samples appear representative of the uncertainty of each input parameter. Such samples are plotted
Arrhenius reaction constants

As for the Arrhenius reaction constants, \( A \) and \( E_a \) must be positive, and as such are specified with gamma distributions. The reaction order \( n \) must be greater than 1.0 for the model to run properly, and as such a triangular distribution is used for it.

The activation energy value determined in Chapter 4 is used as the mean value in its distribution. To determine the standard deviation, the sample standard deviation of the five values obtained via the five slopes shown in Figure 4.5 is used.

For the pre-exponential constant, the standard deviation is determined by calculating five optimal \( A \) values to fit each of the five degradation curves shown in Figure 4.4. The sample standard deviation of these five values is then calculated.

For the reaction order \( n \), the value must be greater than 1.0. A triangular
Figure 5.5: Thermophysical constants—PDFs
distribution is selected, with $a = 1.0$, $b = 1.5$, and $c = 1.01$. It is noted that the mean of this distribution is $1.17 \neq 1.14$, that is the mean of the distribution is not equal to the value determined in Chapter 4. These PDFs are presented in Figure 5.6.

**Mass densities, heat of decomposition, and boundary condition parameters**

Triangular distributions are likewise defined for the mass densities of char and virgin composite, as these are known to within tightly restricted ranges. The heat of decomposition is represented with a normal distribution, as it can switch signs. In the code it is represented as a positive number, which is then changed to negative as it is implemented in the thermal model. The mean and standard deviation are determined for a uniform distribution ranging from $a = 595000$ to $b = 800000$, and then applied to a normal distribution, $\mu = (a + b)/2$ and $\sigma = \sqrt{\frac{1}{12}(b - a)^2}$.

The surface emissivities and convection heat transfer coefficients are described with gamma distributions, as these will not become negative. These distributions are provided in Figure 5.7.

**Summary**

Specific distributions for all variables are defined in Table 5.1. Note that gamma distributions are defined by the parameters $\alpha$ and $\beta$, which may be obtained via the values given in the Table 5.1 as $\beta = \sigma^2/\mu$, and $\alpha = \mu/\beta$. 

Figure 5.6: Arrhenius reaction constants—PDFs
Figure 5.7: Mass densities, heat of decomposition, and thermal boundary condition input parameters—PDFs
Table 5.1: Input variable probability distribution functions

<table>
<thead>
<tr>
<th>Input parameter</th>
<th>Distribution</th>
<th>Distribution parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>Gamma</td>
<td>$\mu = 2.1768 \times 10^{11}, \sigma = 3.0381 \times 10^{10}$</td>
</tr>
<tr>
<td>$c_{pchb}$</td>
<td>Normal</td>
<td>$\mu = 1151.6, \sigma = 15$</td>
</tr>
<tr>
<td>$c_{pchm}$</td>
<td>Normal</td>
<td>$\mu = 0.259, \sigma = 0.06$</td>
</tr>
<tr>
<td>$c_{pgh}$</td>
<td>Normal</td>
<td>$\mu = 2246, \sigma = 200$</td>
</tr>
<tr>
<td>$c_{pgm}$</td>
<td>Normal</td>
<td>$\mu = 2546, \sigma = 750$</td>
</tr>
<tr>
<td>$c_{pwb}$</td>
<td>Normal</td>
<td>$\mu = 1099.3, \sigma = 2.0$</td>
</tr>
<tr>
<td>$c_{pwm}$</td>
<td>Normal</td>
<td>$\mu = 0.0452, \sigma = 0.01$</td>
</tr>
<tr>
<td>$E_a$</td>
<td>Gamma</td>
<td>$\mu = 1.6758 \times 10^4, \sigma = 13768$</td>
</tr>
<tr>
<td>$\epsilon_c$</td>
<td>Gamma</td>
<td>$\mu = 0.01, \sigma = 0.01$</td>
</tr>
<tr>
<td>$\epsilon_h$</td>
<td>Gamma</td>
<td>$\mu = 0.94, \sigma = 0.02$</td>
</tr>
<tr>
<td>$k_{chb}$</td>
<td>Normal</td>
<td>$\mu = 0.2157, \sigma = 0.02$</td>
</tr>
<tr>
<td>$k_{chm}$</td>
<td>Normal</td>
<td>$\mu = 2.83 \times 10^{-4}, \sigma = 6.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>$k_{sc}$</td>
<td>Gamma</td>
<td>$\mu = 1.0, \sigma = 1.0$</td>
</tr>
<tr>
<td>$k_{sh}$</td>
<td>Gamma</td>
<td>$\mu = 7.0, \sigma = 1.5$</td>
</tr>
<tr>
<td>$k_{vwb}$</td>
<td>Normal</td>
<td>$\mu = 0.3308, \sigma = 0.01$</td>
</tr>
<tr>
<td>$k_{vwm}$</td>
<td>Normal</td>
<td>$\mu = 4.404 \times 10^{-5}, \sigma = 1.5 \times 10^{-5}$</td>
</tr>
<tr>
<td>$n$</td>
<td>Triangular</td>
<td>$a = 1, b = 1.5, c = 1.01$</td>
</tr>
<tr>
<td>$Q$</td>
<td>Normal</td>
<td>$\mu = 6.98 \times 10^4, \sigma = 5.92 \times 10^4$</td>
</tr>
<tr>
<td>$\rho_{eh}$</td>
<td>Triangular</td>
<td>$a = 1230, b = 1311, c = 1235$</td>
</tr>
<tr>
<td>$\rho_v$</td>
<td>Triangular</td>
<td>$a = 1680, b = 1800, c = 1683$</td>
</tr>
</tbody>
</table>
Table 5.2: Assumed input parameter correlation coefficients

<table>
<thead>
<tr>
<th>1st parameter</th>
<th>2nd parameter</th>
<th>Correlation coeff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_a$</td>
<td>$n$</td>
<td>0.999</td>
</tr>
<tr>
<td>$A$</td>
<td>$n$</td>
<td>0.977</td>
</tr>
<tr>
<td>$A$</td>
<td>$E_a$</td>
<td>0.974</td>
</tr>
<tr>
<td>$\rho_{ch}$</td>
<td>$\rho_v$</td>
<td>0.75</td>
</tr>
<tr>
<td>$c_{pchb}$</td>
<td>$c_{pveh}$</td>
<td>0.5</td>
</tr>
<tr>
<td>$k_{chb}$</td>
<td>$k_{vb}$</td>
<td>0.5</td>
</tr>
<tr>
<td>$c_{pchm}$</td>
<td>$c_{pem}$</td>
<td>0.25</td>
</tr>
<tr>
<td>$k_{chm}$</td>
<td>$k_{vm}$</td>
<td>0.25</td>
</tr>
<tr>
<td>$c_{pchb}$</td>
<td>$\rho_{ch}$</td>
<td>0.25</td>
</tr>
<tr>
<td>$c_{pveh}$</td>
<td>$\rho_v$</td>
<td>0.25</td>
</tr>
<tr>
<td>$c_{pveh}$</td>
<td>$\rho_{ch}$</td>
<td>0.125</td>
</tr>
</tbody>
</table>

Correlations

Correlations between input parameters in large part were not available, and were therefore only roughly estimated. Per the thermogravimetric data described earlier, $A$ and $n$ values were determined via optimization for the five $E_a$ values resulting from Figure 4.5. That is, for each $E_a$ value, corresponding $A$ and $n$ values were determined. The correlation coefficients between the values are then determined to be 0.974 between $A$ and $E_a$, 0.977 between $A$ and $n$, and 0.999 between $E_a$ and $n$.

Multiple independent data sets for the other properties were not available. As these values are expected to be correlated, correlation coefficients were estimated. All correlation coefficients used are provided in Table 5.2.

5.5.2 Sampling technique

Random numbers for sampling were chosen using Matlab’s internal generator. To determine which sampling technique to employ, random (Monte Carlo) sampling as well as Latin hypercube sampling (LHS, see for instance [36]) were evaluated. LHS was shown to be more efficient than random sampling [49]. Multiple samples were therefore generated therefore using LHS. Once sampling was complete, rank
correlations were enforced upon the sample set using a technique by Iman and Conover [41]. This final set of samples was then run through the model one by one, and the input and output variable values for each sample were recorded for further analysis.

### 5.6 Uncertainty analysis

The Monte Carlo analysis results may be used to conduct an uncertainty analysis to characterize the uncertainty in the model output resulting from the defined uncertainties in the model input. A plot of the variation in the thermal evolution is shown in Figure 5.8. This variation occurs for a thirty-two sample Latin hypercube (fewer samples are used to yield a more intelligible depiction). This shows the likely variability in the temperature evolution resulting from the defined uncertainty in the input parameters. A percentile plot of the data for the 512 samples Latin hypercube yields a more clear depiction of the character of temperature evolution variability, and is provided in Fig. 5.9.

![Figure 5.8: Variation of thermal evolution, thirty-two samples](image-url)
Figure 5.9: Thermal evolution percentile plot, 512 samples. The top line group is at the hot face (HF), the next highest is $1/10^{th}$ of the thickness from the HF, the next is at the panel midpoint, and the lowest line group is at the cold face.

For any particular data set, for instance the temperature data at 1000 seconds and at the skin’s cold face, the output uncertainty may be plotted in the form of a probability distribution function, a cumulative distribution function (CDF), or an inverse cumulative distribution function. Each fully characterizes the uncertainty in that data set. CDFs for a 2048 sample Latin hypercube data set, namely the cold face temperature at 500, 1000, 1500, and 2000 seconds, are shown in Figures 5.10 and 5.11.

5.7 Global sensitivity analysis

The simplest method for performing sensitivity analysis on the Monte Carlo simulation data is to simply plot the various input parameter values vs. the various output parameter values. If the particular input parameter has a significant effect on the output variable, to the extent that this relationship can be seen through the variations of all of the other input parameters, than this relationship will be
Figure 5.10: Empirical cumulative distribution function, mean (value noted), and
distribution function (histogram), for 2048 sample Latin hypercube data. The
specific data set is the cold face temperature at time $t = 500$ s (left), and $t = 1000$ s
(right).

Figure 5.11: Empirical cumulative distribution function, mean (value noted), and
distribution function (histogram), for 2048 sample Latin hypercube data. The
specific data set is the cold face temperature at time $t = 1500$ s (left), and $t = 2000$ s (right).

visible in these scatterplots. Even rather complex nonlinear relationships may be
determined in this manner. Scatterplots for the current model are provided in
Figures 5.12–5.17.

Of these, clear relationships are only visible for $c_{pgb}$ and the Arrhenius reaction
parameters. Clearly the uncertainty in $c_{pgb}$ has a significant effect on the model
output, and increasing its value decreases the expected temperature. With regard
to the Arrhenius reaction parameters, there appears to be a very strong relation-
ship between these input parameters and the resulting temperature prediction.
Figure 5.12: Scatterplots. The input parameters are (clockwise from top-left) intercept and slope values for the specific heat of the char, and slope and intercept values for the specific heat of the virgin composite. The output variable is cold face temperature at time $t = 1000$ s.

Figure 5.13: Scatterplots. The input parameters are the intercept (left) and slope (right) values for the specific heat of the pyrolysis gases; the output variable is cold face temperature at time $t = 1000$ s.
Figure 5.14: Scatterplots. The input parameters are (clockwise from top-left) intercept and slope values for the thermal conductivity of the char, and slope and intercept values for the thermal conductivity of the virgin composite. The output variable is cold face temperature at time $t = 1000$ s.

Figure 5.15: Scatterplots. The input parameters are (from left) the pre-exponential constant, the activation energy, and the reaction order; the output variable is cold face temperature at time $t = 1000$ s.
Figure 5.16: Scatterplots. The input parameters are (from left) the mass density of the char, mass density of the virgin composite, and heat of decomposition; the output variable is cold face temperature at time \( t = 1000 \) s.

Figure 5.17: Scatterplots. The input parameters are (clockwise from top-left) surface emissivity of cold and hot faces, and convective heat transfer coefficients of hot and cold faces. The output variable is cold face temperature at time \( t = 1000 \) s.
However, per Helton, “inclusion of multiple correlated input parameters can lead to regression coefficients that do not reflect the importance of the individual variables” [35]. It is therefore believed that the very strong correlations between these three variables which were imposed on the samples led to them having influence beyond what they would have individually.

Now more quantitative estimators of sensitivity will be introduced. The sampled input parameter values and corresponding output variable values resulting from the Monte Carlo analysis may also be used to apportion the uncertainty in the thermal output to the individual input parameters. Global sensitivity estimators do exactly this. Various estimators of global sensitivity are available, among them Pearson and Spearman coefficients, standardized regression and standardized rank regression coefficients, and partial correlation and partial rank correlation coefficients. In the following discussion, these estimators are first defined, and then the most useful are described in more detail and applied to the current model.

A model may be thought of as a mapping from a set of input parameters \( (x_k) \) to a set of output data \( (y) \). A similar mapping between the input parameters and the output variables of the form

\[
\hat{y} = b_0 + \sum_{k=1}^{n} b_k x_k \quad (5.5)
\]

may be obtained using a least squares regression. Here \( n \) is the number of input parameters. In matrix form, this is

\[
y = Xb, \quad (5.6)
\]

where

\[
y = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_{11} & \ldots & x_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{m1} & \ldots & x_{mn} \end{bmatrix}, \quad b = \begin{bmatrix} b_0 \\ \vdots \\ b_n \end{bmatrix}. \quad (5.7)
\]

Here \( m \) is the number of samples. The regression coefficients \( b \) are then given by:

\[
b = (X^T X)^{-1} X^T y. \quad (5.8)
\]
The standardized regression coefficients (SRCs) measure the effect of varying each parameter by a given fraction of its standard deviation, with others held constant. They are given by \( b_k \hat{s}_{x_k} / \hat{s}_y \), with \( b_k \) the regression coefficients just defined, normalized by the ratio of \( \hat{s}_{x_k} \) to \( \hat{s}_y \), which are the sample standard deviations of the input and output variables, respectively,

\[
\hat{s}_y = \left[ \sum_{i=1}^{m} \frac{(y_i - \bar{y})^2}{m-1} \right]^{1/2}, \quad \hat{s}_{x_k} = \left[ \sum_{i=1}^{m} \frac{(x_{ki} - \bar{x}_k)^2}{m-1} \right]^{1/2}.
\] (5.9)

The correlation coefficient, or Pearson correlation, measures the quality of a least squares regression such as (5.5). The correlation coefficient \( r_{x_ky} \) between \( x_k \) and \( y \) is given by

\[
r_{xy} = \frac{\sum_{i=1}^{m} (x_{ki} - \bar{x}_k)(y_i - \bar{y})}{\left[ \sum_{i=1}^{m} (x_{ki} - \bar{x}_k)^2 \right]^{1/2} \left[ \sum_{i=1}^{m} (y_i - \bar{y})^2 \right]^{1/2}},
\] (5.10)

where \( \bar{x}_k \) indicates the mean value of \( x_k \). In general, correlation coefficients range from 1.0 to −1.0. A value of 1.0 indicates a direct linear correlation, a value of 0.0 no correlation, and a value of −1.0 a inverse linear correlation.

The square of the correlation coefficient, or coefficient of determination \( r^2 \), gives the quality of the least squares fit. It ranges from 0.0 to 1.0: a value of 1.0 indicates that the regression fully accounts for the variability in the data, and a value of 0.0 indicates that the least squares regression doesn’t account for any of this variability.

The partial correlation coefficient (PCC) measures the quality of the least squares regression between an output variable and an individual input parameter, after correcting for the effects of the other input parameters. To determine its value, two linear regression models are constructed, one the given input parameter as a function of all other input parameters, the other the output variable as a function of the other input parameters:

\[
\hat{x}_k = c_0 + \sum_{j=1 \atop j \neq k}^{n} c_j x_j, \quad \hat{y} = b_0 + \sum_{j=1 \atop j \neq k}^{n} b_j x_j.
\] (5.11)
The partial correlation coefficient \( p_{x_ky} \) is the correlation coefficient between \( x_k - \hat{x}_k \) and \( y - \hat{y} \).

In general, SRCs are relatively sensitive to the distribution chosen to represent the input parameter. They are also influenced significantly by the magnitude of the impact the input parameter has on the output variable. The PCCs on the other hand tend not to be affected by the distribution chosen for the input parameter, the magnitude of the impact the input parameter has on the output variable, or the effects of other variables. Note that if the input parameters are uncorrelated, the rank order of input parameter importance resulting from either SRCs or PRCs would be the same [35].

SRCs and PCCs are based on developing linear relationships between the input and output variables. For nonlinear models, this can lead to poor results. A method used to overcome this is to use rank-transformed data in place of the original values—that is, to replace the data with their respective rank in the sample set, and with an average rank assigned to equivalent numbers. In particular, the smallest value receives the rank of 1, and the largest value the rank \( m \). The standardized rank regression coefficients (SRRCs) are the SRCs calculated using rank-transformed data, the Spearman correlation is the Pearson correlation determined with rank-transformed data, and the partial rank correlation coefficients (PRCCs) are the PCCs obtained with the rank-transformed data set. The calculation of these estimators from rank-transformed data determines the strength of monotonic relationships between the original data, as opposed to the strength of linear relationships between those data.

It is noted that Saltelli and Marivoet report a study of various global sensitivity parameters, including those discussed herein [72]. The parameters were applied to a nonlinear model and the results compared. Among their conclusions was that the PRCC and SRRC estimators appeared to be, in general, the most robust and reliable. Figures 5.18, 5.19, 5.21, and 5.22 provide the SRRCs and PRCCs resulting from the Monte Carlo data. Figures 5.20 and 5.23 provide the rank order of the absolute values of these coefficients.

Note that the \( r^2 \) statistic (coefficient of determination) for the SRRC regressions
Figure 5.18: Standardized rank regression coefficients. The input parameters are listed, the output variable is midpoint (top) and cold face (bottom) temperature. The values throughout the evolution of the problem are displayed for each input parameter.
Figure 5.19: Standardized rank regression coefficients. The input parameters are listed, the output variable is near-cold face mass density. The values throughout the evolution of the problem are displayed for each input parameter.

(temperature at cold face) at each time step range from 0.640 to 0.992, indicating that these coefficients in the current application account for a large proportion of the estimated uncertainty.

### 5.8 Comparison of local and global SA results

The results for the local and global SA at the panel midpoint and cold face in many ways agree, yet also contrast in a few instances. The three measures are in agreement that $c_{pgb}$, $E_a$, $k_{chb}$, and $\rho_e$ are very important throughout the simulation; and that $k_{vb}$ is very important at the beginning of the simulation. They agree that $k_{chm}$ and $\rho_{ch}$ are quite important throughout of the simulation, and $\epsilon_h$ is quite important at the end of the simulation. They agree that the parameters $A$, $c_{pgm}$, $c_{pvh}$, $c_{pvm}$, $k_{vm}$, $n$, and $Q$ are less important. Finally, they agree that $c_{pchm}$, $c_{pchb}$, and $k_{sh}$ are unimportant.

The significant difference between the two results is in $\epsilon_c$ and $k_{sc}$—these are important in the global SA, while being unimportant in the local SA. Global SA apportions the output variable uncertainty to the individual input parameters. Table 5.3 provides the coefficient of variation for each of the input parameters. This is simply the standard deviation of the distribution divided by the mean.
Figure 5.20: Rank order of absolute value of standard rank regression coefficients with time. The input parameters are listed, the output variable is midpoint (top) and cold face (bottom) temperature.
Figure 5.21: Partial rank correlation coefficients. The input parameters are listed, the output variable is midpoint (top) and cold face (bottom) temperature. The values throughout the evolution of the problem are displayed for each input parameter.
Figure 5.22: Partial rank correlation coefficients. The input parameters are listed, the output variable is near-cold face mass density. The values throughout the evolution of the problem are displayed for each input parameter.

Table 5.3: Coefficient of variation for input parameter distributions

<table>
<thead>
<tr>
<th>Input parameter</th>
<th>Coefficient of variation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>$c_v = 14.0%$</td>
</tr>
<tr>
<td>$c_{pchb}$</td>
<td>$c_v = 1.3%$</td>
</tr>
<tr>
<td>$c_{pchm}$</td>
<td>$c_v = 23%$</td>
</tr>
<tr>
<td>$c_{pgb}$</td>
<td>$c_v = 8.9%$</td>
</tr>
<tr>
<td>$c_{pgm}$</td>
<td>$c_v = 30%$</td>
</tr>
<tr>
<td>$c_{pvm}$</td>
<td>$c_v = 0.182%$</td>
</tr>
<tr>
<td>$c_{pvp}$</td>
<td>$c_v = 22%$</td>
</tr>
<tr>
<td>$E_a$</td>
<td>$c_v = 8.2%$</td>
</tr>
<tr>
<td>$\epsilon_e$</td>
<td>$c_v = 100%$</td>
</tr>
<tr>
<td>$\epsilon_h$</td>
<td>$c_v = 21%$</td>
</tr>
<tr>
<td>$k_{chb}$</td>
<td>$c_v = 9.3%$</td>
</tr>
<tr>
<td>$k_{chm}$</td>
<td>$c_v = 21%$</td>
</tr>
<tr>
<td>$k_{sc}$</td>
<td>$c_v = 100%$</td>
</tr>
<tr>
<td>$k_{sh}$</td>
<td>$c_v = 21%$</td>
</tr>
<tr>
<td>$k_{vb}$</td>
<td>$c_v = 3.0%$</td>
</tr>
<tr>
<td>$k_{vm}$</td>
<td>$c_v = 34%$</td>
</tr>
<tr>
<td>$n$</td>
<td>$c_v = 10.0%$</td>
</tr>
<tr>
<td>$Q$</td>
<td>$c_v = 8.5%$</td>
</tr>
<tr>
<td>$\rho_{ch}$</td>
<td>$c_v = 1.47%$</td>
</tr>
<tr>
<td>$\rho_v$</td>
<td>$c_v = 1.62%$</td>
</tr>
</tbody>
</table>
Figure 5.23: Rank order of absolute value of partial rank correlation coefficients with time. The input parameters are listed, the output variable is midpoint (top) and cold face (bottom) temperature.
value. A large coefficient of variation indicates large input parameter uncertainty. The two variables with the highest coefficient of variation are not surprisingly $\epsilon_c$ and $k_{sc}$. This explains why they gain importance in the global estimators, yet lose importance in the local estimators. In general, a relatively large coefficient of variation increases the global estimator values with respect to the local, while a small coefficient of variation decreases the global estimator values with respect to the local.

As well, the sign of the coefficients are nearly identical between the local and global analyses, except for the value of $Q$. In the local SA, the coefficients for $Q$ are negative, while in the global SA they are positive. This may be explained by the fact that the value of $Q$ is negative (i.e. the reaction is endothermic), and therefore in the local SA, the normalization of the sensitivity coefficient results in multiplication by a negative number thereby changing the sign. With these few discrepancies thus explained, the agreement between the two analyses is indeed quite satisfactory.

### 5.9 Validation

The temperature evolution that results from running the thermal model using the input parameters specified in Section 5.4 is given in Figure 5.24. Clearly there is a significant difference between the predicted and measured temperatures, though the overall behavior is captured quite well by the model. The goal of this section is to determine whether or not the expected variability within the input parameters is enough to explain this difference, or if instead the difference exceeds this uncertainty and therefore must result from the inadequacy of the thermal model itself.

To validate the present technique, a 512 sample Monte Carlo simulation was run. These 512 samples were then scored in comparison with experimental results obtained via Lattimer and Ouellette [50]. The score to minimize was the largest singular value norm of the difference between the experimental temperatures and the calculated temperatures throughout the simulation. The samples were then
Figure 5.24: Predicted temperatures vs. experimentally measured temperatures

The twenty input variable values for each sample were then examined. The goal was to find the optimum result that didn’t contain relatively improbable input parameter values. The lowest-scoring sample for which all input parameter values were within the 10<sup>th</sup> and 90<sup>th</sup> percentiles is also included in Table 5.4. The temperatures which result from both samples are shown in Figure 5.25.

As a result of this validation exercise, one might conclude that the expected variability within the input parameter values could indeed account for much of the difference between the predicted and experimentally measured temperature values.

### 5.10 Conclusions

Sensitivity analyses and an uncertainty analysis of a model for the pyrolytic decomposition of and heat transfer through a composite panel have been performed herein, and the model has been validated using this data. The local sensitivities of this thermal model to its input parameters are first determined. Then the uncertainty in the thermal output resulting from a defined set of uncertain input data is estimated. This uncertainty is apportioned to the individual input parameters in
Table 5.4: Sampled input parameter values that result in optimal match between predicted temperatures and experimentally measured temperatures.

<table>
<thead>
<tr>
<th>Input parameter</th>
<th>Optimal sample value</th>
<th>Likely optimal value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>$1.72 \times 10^{11}$</td>
<td>$1.83 \times 10^{11}$</td>
</tr>
<tr>
<td>$c_{pchb}$</td>
<td>1160</td>
<td>1171</td>
</tr>
<tr>
<td>$c_{pchem}$</td>
<td>0.297</td>
<td>0.205</td>
</tr>
<tr>
<td>$c_{pgb}$</td>
<td>1586</td>
<td>1948</td>
</tr>
<tr>
<td>$c_{pgm}$</td>
<td>2380</td>
<td>3510</td>
</tr>
<tr>
<td>$c_{pwb}$</td>
<td>1101</td>
<td>1102</td>
</tr>
<tr>
<td>$c_{pvm}$</td>
<td>0.0498</td>
<td>0.0408</td>
</tr>
<tr>
<td>$E_a$</td>
<td>147900</td>
<td>151600</td>
</tr>
<tr>
<td>$e_c$</td>
<td>0.00268</td>
<td>0.001102</td>
</tr>
<tr>
<td>$e_h$</td>
<td>0.927</td>
<td>0.927</td>
</tr>
<tr>
<td>$k_{chb}$</td>
<td>0.1969</td>
<td>0.237</td>
</tr>
<tr>
<td>$k_{chm}$</td>
<td>$2.73 \times 10^{-4}$</td>
<td>$3.31 \times 10^{-4}$</td>
</tr>
<tr>
<td>$k_{sc}$</td>
<td>1.468</td>
<td>0.819</td>
</tr>
<tr>
<td>$k_{sh}$</td>
<td>7.86</td>
<td>5.70</td>
</tr>
<tr>
<td>$k_{vwb}$</td>
<td>0.333</td>
<td>0.329</td>
</tr>
<tr>
<td>$k_{vwm}$</td>
<td>$4.28 \times 10^{-5}$</td>
<td>$3.77 \times 10^{-5}$</td>
</tr>
<tr>
<td>$n$</td>
<td>1.024</td>
<td>1.035</td>
</tr>
<tr>
<td>$Q$</td>
<td>$-642000$</td>
<td>$-659000$</td>
</tr>
<tr>
<td>$\rho_{ch}$</td>
<td>1282</td>
<td>1254</td>
</tr>
<tr>
<td>$\rho_v$</td>
<td>1775</td>
<td>1698</td>
</tr>
</tbody>
</table>
Figure 5.25: Optimal solution (top), and optimal probable solution (bottom); both from 512 sample simulation.
a global sensitivity analysis. Finally, validation of the model using the uncertain thermal output is performed.

These analyses reveal how the model result is affected by the individual input parameter values. This is shown for instance in Fig. 5.1, in which a positive sensitivity coefficient indicates that increasing the input parameter value leads to an increase in predicted temperature, and the magnitude of the coefficient indicates the scale of the variation in predicted temperature. As experimental thermal data is measured directly, any differences between that data and the model prediction may be explained using these results. For instance, if the thermal result fits within the bounds determined in the uncertainty analysis, but does not match the predicted temperature evolution, an educated guess may be formulated as to which input parameter might be erroneous thus precluding accurate modeling.

The relative importance of various input parameters can also be determined using for instance Figures 5.3, 5.20, and 5.23. These figures reveal that the input parameters \( c_{pgb}, E_a, k_{chb} \), and \( \rho_v \) are very important throughout the simulation; and that \( k_{vb} \) is very important at the beginning of the simulation. They show that \( k_{chm} \) and \( \rho_{ch} \) are quite important throughout the simulation, and \( \epsilon_h \) is quite important at the end of the simulation. They further show that the parameters \( A, c_{pgm}, c_{pvb}, c_{pvm}, k_{vm}, n, \) and \( Q \) are less important. Finally, they show that \( c_{pchm}, c_{pchb}, \) and \( k_{sh} \) are unimportant, and expending great effort in accurately determining their value is unnecessary and would not yield a significant improvement in the accuracy of the predicted temperature values.

The uncertainty in the predicted thermal evolution is shown for instance in Figure 5.9. This provides an estimate of the expected range of experimental values likely to be observed. As well, it indicates the degree of confidence one might have in the predicted thermal result. Again, these results must be viewed with the limitations of the current model (i.e. does not account for gas accumulation, pressurization, expansion, etc.) in mind. As well, the statistical distributions used to represent the uncertainty in the input parameters are hypothesized based on the limited experimental data available at this time, again limiting the value of these results.
5.11 Acknowledgements

Chapter 5, in part, is a reprint of text appearing in a paper by W. T. Ramroth, P. Krysl, and R. J. Asaro; entitled “Sensitivity and Uncertainty Analyses for FE Thermal Model of FRP Panel Exposed to Fire”; *Compos Part A: Appl S* 37(7):1082–91, 2006. The dissertation author was the primary author of this material.
Chapter 6

Thermal deflection model

6.1 Introduction

This chapter represents a small detour from the prevailing theme of the overall dissertation. In this chapter, a separate model for determining the thermal deflection of a pin-pin rectangular panel exposed to fire is determined (other boundary conditions may be easily obtained from the results herein). The model, and its numerical implementation, account for an arbitrary gradation both in temperature, elastic modulus, and coefficient of thermal expansion through the panel (in through-the-thickness direction).

This model has proven useful for predicting the thermal deflections that will be observed in test specimens. It also will be shown to provide a method for determining a minimum fraction for the degraded elastic constant—something that will be discussed in more detail in Chapter 8. This parameter in fact is a critical unknown in the present methodology—thus this observation could prove to be of value.

The chapter will begin with a brief discussion of the degradation of the elastic modulus in FRP composites with exposure to elevated temperature. This behavior will then be used to yield an elasticity solution for the temperature-dependent coefficient of thermal expansion of an FRP composite material. The model for the out-of-plane thermal deflection of a pin-pin beam with varying temperature, elastic modulus, and coefficient of thermal expansion profiles will then be introduced.
Finally, an example application of the model will be discussed.

6.2 Degradation of elastic constants with temperature

The variation in mechanical properties of FRP composites with exposure to elevated temperatures will be discussed in more detail in Chapter 8. This section provides a brief introduction such that the basic principles can be used in the development of the present model.

The degradation of the mechanical properties of FRP composites with exposure to elevated temperatures is governed by the glass transition that these materials pass through, as discussed in Section 1.4.3. In particular, at the glass transition temperature, the matrix resin transitions from a glassy (brittle) state to a rubbery (pliable) state. For the E-glass/vinylester composite of interest in the present application, this transition can be seen in Figure 1.1, and is shown therein to take place at around 125°C.

As the composite approaches this glass transition temperature, the matrix resin loses its strength, and thus its ability to hold the fibers in place and transfer load between them. As a result, one might expect the composite to lose most if not all of its strength, at least in compression, as the glass transition temperature is reached. Actual data are available, and are presented in Figure 6.1, together with a curve fit to all of these various data points.

The fitted curves shown in Figure 6.1 (specified numerically in Chapter 8) provide the temperature-dependent elastic modulus of the FRP composite and core materials (for a sandwich panel). The elastic modulus throughout the panel is given by

$$E(x) = f(T(x)) \cdot E$$

where $T(x)$ is the through-the-panel temperature profile, $f(T(x))$ is the material property fraction at $T(x)$ resulting from the relations plotted in Figure 6.1, and $E$ is the undegraded elastic modulus.
Figure 6.1: Fraction of mechanical properties with temperature (minimum fraction $X/X_0 = 0.01$).

### 6.3 Elasticity solution for temperature-dependent coefficient of thermal expansion of FRP composite material

In this section, an elasticity solution for the temperature-dependent coefficient of thermal expansion of an arbitrary FRP composite material is determined. This will be derived using an equilibrium equation, a compatibility equation, and a constitutive equation.

To begin, assume that an FRP composite panel is exposed to an elevated temperature profile. The fibers and the matrix resin will both expand/contract due to the temperature change, and will likely do so in differing amount, such that an internal force couple develops between the two. As the panel is still in static equilibrium, these two forces must be in equilibrium. Assume that the fibers expand more than the matrix, for instance—in this case, the matrix will subject the fibers to a force that serves to restrain their expansion, and the expanding fibers will exert a force on the matrix that is equal to the counteracting force but
opposite in direction. Thus,

\[
F_f = -F_m \\
\sigma_f A_f = -\sigma_m A_m \\
\sigma_f V_f A = -\sigma_m (1 - V_f) A \\
\sigma_f V_f = -\sigma_m (1 - V_f) \\
\sigma_f = -\sigma_m \frac{1 - V_f}{V_f}
\]  

(6.2)

Herein \(F\) is the force, \(\sigma\) the stress, and \(A\) the area. The subscript \(f\) indicates fiber, and the subscript \(m\) indicates matrix resin. \(V_f\) indicates the volume fraction of fiber (thus \(V_m = 1 - V_f\) would be the volume fraction of matrix resin).

The next step is to utilize assumed elastic constitutive properties of the matrix and fiber. Thus,

\[
\epsilon_{\text{mech.}}^f = \frac{\sigma_f}{E_f} \\
\epsilon_{\text{mech.}}^m = \frac{\sigma_m}{E_m}
\]  

(6.3)

Herein \(\epsilon\) is the strain, and \(E\) the elastic modulus. The superscript “mech.” indicates the mechanical strain is referred to.

The final step is to use a compatibility equation. The strain within the fibers is known to be compatible with the strain within the matrix. Thus the two strains may be equated, and bringing in the equilibrium equation and the constitutive relations, the following is obtained:

\[
\epsilon_f = \epsilon_m \\
\epsilon_f^{\text{therm.}} + \epsilon_f^{\text{mech.}} = \epsilon_m^{\text{therm.}} + \epsilon_m^{\text{mech.}} \\
\alpha_f \Delta T + \frac{\sigma_f}{E_f} = \alpha_m \Delta T + \frac{\sigma_m}{E_m} \\
\alpha_f \Delta T - \frac{\sigma_m (1 - V_f)}{E_f V_f} = \alpha_m \Delta T + \frac{\sigma_m}{E_m} \\
\Delta T (\alpha_f - \alpha_m) = \sigma_m \left( \frac{1}{E_m} + \frac{1 - V_f}{E_f V_f} \right) \\
\Delta T (\alpha_f - \alpha_m) = \sigma_m \left( \frac{E_f V_f + E_m (1 - V_f)}{E_f E_m V_f} \right) \\
\sigma_m = \Delta T (\alpha_f - \alpha_m) \left( \frac{E_f E_m V_f}{E_f V_f + E_m (1 - V_f)} \right)
\]  

(6.4)
Here $\alpha$ indicates the coefficient of thermal expansion, and $\Delta T$ indicates the temperature change (from ambient).

But as has been shown previously,

$$\epsilon = \epsilon_m = \alpha_m \Delta T + \frac{\sigma_m}{E_m}.$$  

So from the definition of the coefficient of thermal expansion we have

$$\alpha = \frac{\epsilon}{\Delta T} = \frac{\alpha_m \Delta T + \frac{\sigma_m}{E_m}}{\Delta T} = \alpha_m + \frac{\sigma_m}{E_m \Delta T}$$

$$\alpha = \alpha_m + (\alpha_f - \alpha_m) \left( \frac{E_f V_f}{E_f V_f + E_m (1 - V_f)} \right)$$  

(6.5)

As the FRP composite rises in temperature, the elastic modulus of the fiber will stay constant while the elastic modulus of the matrix resin will degrade as discussed in Section 6.2. Thus a thermally-dependent coefficient of thermal expansion for the FRP composite material may be obtained by reducing the value of $E_m$ in Equation (6.5) according to Equation (6.1). Thus the coefficient of thermal expansion as varies in the through-the-panel direction is obtained as

$$\alpha(x) = \alpha_m + (\alpha_f - \alpha_m) \left( \frac{E_f V_f}{E_f V_f + E_m(x) (1 - V_f)} \right)$$  

(6.6)

where $E_m(x)$ is given by Equation (6.1). Note that this $x$ indicates variation in the through-the-panel direction. In the next section a separate coordinate system will be introduce which contradicts this directly. Please note that the coordinate system introduced in the following section is limited in scope to that section only.

### 6.4 Thermal deflections

In this section an elasticity solution for the thermal deflection of a pin-pin rectangular panel with arbitrarily varying temperature, elastic constant, and coefficient
of thermal expansion profiles in the through-the-thickness direction. As such, the model will inherently represent the behavior of any single or sandwich panel configuration. Deflections for some other boundary conditions may be determined from this result in a very straightforward manner.

The method followed is adapted from the work of Boley and Weiner [12]. In particular, the work of Boley assumes that the panel has constant elastic modulus and coefficient of thermal expansion, but is non-rectangular. In the present work the variable material properties complicate the derivation, while the geometric assumption provides for simplification.

The method uses a system of centroidal axes, or in other words the origin of the coordinate system used is located at the centroid of the panel. The axes used are shown in Figure 6.2. Please note that this coordinate system directly contradicts the coordinate system used throughout the rest of the dissertation, and is only relevant to the discussion within this section.

This method assumes the panel behaves as a beam, in accordance with the common Euler-Bernoulli assumptions (plane sections remain plane, etc.). As a result the axial displacement $u$ will be linear with respect to $y$ (note that there is no variation in the $z$ direction), i.e. of the form

$$u = f_0(x) + y f_1(x).$$

(6.7)
Using the strain-displacement relation and the elastic constitutive relation we have

\begin{align*}
\varepsilon_{xx} &= \frac{\partial u}{\partial x} = f'_0(x) + y f'_1(x) \\
\sigma_{xx} &= E(y) (\varepsilon_{xx} - \alpha(y) \Delta T(y)) \\
\sigma_{xx} &= E(y) (f'_0(x) + y f'_1(x) - \alpha(y) \Delta T(y))
\end{align*}

(6.8)

(6.9)

where it is noted that $E(y)$, $\alpha(y)$ and $\Delta T(y)$ denote that the elastic modulus, coefficient of thermal expansion, and temperature increment are functions of $y$.

The constants $f'_0$ and $f'_1$ must be determined to satisfy equilibrium equations. These equations take the form

\begin{align*}
\int_A \sigma_{xx} \, dA &= 0 \\
\int_A \sigma_{xx} \, y \, dA &= 0
\end{align*}

(6.10)

(6.11)

Substituting Equation (6.9) into Equation (6.10) yields

\begin{align*}
\int_A E(y) (f'_0(x) + y f'_1(x) - \alpha(y) \Delta T(y)) \, dA &= 0 \\
f'_0(x) \int_A E(y) \, dA + f'_1(x) \int_A E(y) \, y \, dA - \int_A \alpha(y) E(y) \Delta T(y) \, dA &= 0
\end{align*}

(6.12)

Substituting Equation (6.9) into Equation (6.11) yields

\begin{align*}
\int_A E(y) (f'_0(x) + y f'_1(x) - \alpha(y) \Delta T(y)) \, y \, dA &= 0 \\
f'_0(x) \int_A E(y) \, y \, dA + f'_1(x) \int_A E(y) \, y^2 \, dA - \int_A \alpha(y) E(y) \Delta T(y) \, y \, dA &= 0
\end{align*}

(6.13)

Equations (6.12) and (6.13) form two equations that may be solved for unknowns $f'_0(x)$ and $f'_1(x)$. 
For ease of consideration, the following integrals are defined:

\[ I_1 = \int_A E(y) \, dA \]
\[ I_2 = \int_A E(y) \, y \, dA \]
\[ I_3 = \int_A E(y) \, y^2 \, dA \]
\[ I_4 = \int_A \alpha(y) \, E(y) \, \Delta T(y) \, dA \]
\[ I_5 = \int_A \alpha(y) \, E(y) \, \Delta T(y) \, y \, dA \]  \hspace{1cm} (6.14)

Note that all of the quantities in these integrals are known, and thus these integrals may be numerically determined directly. The simultaneous equations may then be written

\[ f'_0(x) \, I_1 + f'_1(x) \, I_2 = I_4 \]
\[ f'_0(x) \, I_2 + f'_1(x) \, I_3 = I_5 \]  \hspace{1cm} (6.15)

from which \( f'_0(x) \) and \( f'_1(x) \) are found to be constants defined as

\[ f'_0 = \frac{I_3 \, I_4 - I_2 \, I_5}{I_1 \, I_3 - I_2^2} \]
\[ f'_1 = \frac{I_1 \, I_5 - I_2 \, I_4}{I_1 \, I_3 - I_2^2} \]  \hspace{1cm} (6.16)

Now the axial thermal stresses are fully characterized using Equation (6.9) together with Equations (6.16) and (6.14).

To determine the out-of-plane deflection, consider two cross sections within the panel lying in the planes \( x = x_1 \) and \( x = x_1 + dx_1 \). After temperature changes occur, these planes are assumed to remain plane, and will lie at the following locations, respectively:

\[ x = x_1 + u(x_1, y) \]  \hspace{1cm} (6.17)
\[ x = x_1 + dx_1 + u(x_1, y) + \frac{\partial u}{\partial x_1} \, dx_1 \]  \hspace{1cm} (6.18)

These planes are depicted in Figure 6.3. These two planes (lines in \( x-y \) plane in the present context) meet at the center of curvature of the deflected panel. The
angle between the two lines is defined as $d\alpha_y$. To determine the value of $d\alpha_y$, assume that angles are small, such that the small angle assumption holds (i.e. $\tan(\theta) \approx \sin(\theta) \approx \theta$). Consider the triangles shown in Figure 6.3. The hypotenuse of these triangles travels from $y = 0$ to another arbitrary point on the line at $y = y$. The triangles are right, and the other two sides are parallel to the $x$ and $y$ coordinate directions. With respect to these two triangles, the angle $d\alpha_y$ is given by

$$d\alpha_y = \tan\left(\frac{\Delta x_{x_1+dx_1}}{y}\right) - \tan\left(\frac{\Delta x_{x_1}}{y}\right)$$

$$d\alpha_y \approx \frac{\Delta x_{x_1+dx_1}}{y} - \frac{\Delta x_{x_1}}{y}$$

$$d\alpha_y \approx \frac{1}{y} (\Delta x_{x_1+dx_1} - \Delta x_{x_1})$$

$$d\alpha_y \approx \frac{1}{y} \left( \left( x_{x_1+dx_1}(y = y) - x_{x_1+dx_1}(y = 0) \right) - \left( x_{x_1}(y = y) - x_{x_1}(y = 0) \right) \right)$$

(6.19)
Herein the quantities are given by Equations (6.18) and (6.8). Substituting,

\[
\begin{align*}
d\alpha_y & \approx \frac{1}{y} \left( \left( x_1 + dx_1 + u(x_1, y = y) + (f_0' + y f_1') dx_1 \right) - \\
& \left( x_1 + dx_1 + u(x_1, y = 0) + f_0' dx_1 \right) \right) - \\
& \left( \left( x_1 + u(x_1, y = y) \right) - \left( x_1 + u(x_1, y = 0) \right) \right) \\
\end{align*}
\]

\[
\begin{align*}
d\alpha_y & \approx \frac{1}{y} \left( \left( f_0' + y f_1' \right) dx_1 \right) - \left( f_0' dx_1 \right) \\
d\alpha_y & \approx \frac{1}{y} \left( y f_1' dx_1 \right) \\
d\alpha_y & \approx f_1' dx_1 \\
\end{align*}
\]

(6.20)

But if one considers a triangle from the center of curvature to the center of the deflected panel, the distance between the two will be the radius of curvature \( R_y \).

From geometry (using the assumption of small angles),

\[
\sin(d\alpha_y) \approx \frac{dx_1}{R_y} \\
d\alpha_y \approx \frac{dx_1}{R_y} \\
\frac{1}{R_y} \approx \frac{d\alpha_y}{dx_1} \tag{6.21}
\]

Substituting and simplifying,

\[
\frac{1}{R_y} \approx \frac{f_1' dx_1}{dx_1} = f_1' \tag{6.22}
\]

By definition,

\[
\frac{d^2v}{dx^2} = \frac{1}{R_y} \\
\frac{d^2v}{dx^2} \approx -f_1' \tag{6.23}
\]

Where the negative sign is brought in to yield a correct sign for the deflections. The curvature, given by Equation (6.23) (together with Equations (6.16) and (6.14)), may then be integrated, and boundary conditions brought in, to yield an expression for the thermal deflection.

\[
\frac{d^2v}{dx^2} \approx -f_1' \\
\frac{dv}{dx} \approx -f_1' x + C_1 \tag{6.24}
\]
For the case of pin-pin boundary conditions, \( \frac{dv}{dx} \) at \( x = 0 \) is zero, so \( C_1 = 0 \).

Continuing for the case of pin-pin boundary conditions,

\[
\frac{dv}{dx} \approx -f'_1 x \\
v \approx -f'_1 \frac{x^2}{2} + C_2
\]  

\( (6.25) \)

Again, for pin-pin boundary conditions \( v = 0 \) at \( x = \frac{L}{2} \). Thus \( C_2 = f'_1 \frac{L^2}{8} \), and

\[
v \approx -f'_1 \frac{x^2}{2} + f'_1 \frac{L^2}{8} \\
v \approx f'_1 \left( \frac{L^2}{8} - \frac{x^2}{2} \right)
\]  

\( (6.26) \)

Of course, the maximum deflection will occur at \( x = 0 \), therefore the maximum deflection will be

\[
v_{max} \approx f'_1 \frac{L^2}{8}
\]  

\( (6.27) \)

### 6.5 Example application

In this section, first typical properties for use in this model will be given, and second an example application of the model will be described.

#### 6.5.1 Thermal deflection model properties

The properties which are necessary to run this model include the elastic modulus of the fiber and the undegraded elastic modulus of the resin. The degradation relation used on the resin elastic modulus will be given in Chapter 8. Also required is the fiber volume fraction, and the coefficient of thermal expansion for the fiber and undegraded resin.

Typical values for these properties of e-glass/vinylester composite are available in the literature. A typical elastic modulus (tensile) value for e-glass (and high tensile strength carbon) fibers is specified as 72500 MPa (and 227000 MPa) [33]. A typical undegraded elastic modulus (tensile) for cast vinylester resins is 3300 MPa [45]. Specific values for Derakane 510A-40 vinylester resin are available in the product
literature for this resin, these are similar at 3400 MPa for the tensile modulus and 3600 MPa for the flexural modulus [8].

The coefficient of thermal expansion for e-glass fibers is provided in the literature as $5.0 \times 10^{-6} \text{ m/(m\cdot K)}$ [53]. The value for carbon fiber is given as $-0.5 \times 10^{-6} \text{ m/(m\cdot K)}$ by the same reference. A coefficient of thermal expansion of $5 \times 10^{-5} \text{ m/(m\cdot K)}$ has been recommended for vinylester [4].

Data for various core materials are provided in the product literature [20]. Further data for the Balsa core material are also available [11], in particular this provides elastic constants in the radial and tangential directions that are unavailable in the Diab ProBalsa product literature.

### 6.5.2 Example application

As an example, consider a typical bulkhead panel in a naval ship. The panel is a carbon fiber-reinforced vinylester sandwich with an end-grain balsa core. It is in a pin/pin configuration. The panel is insulated with either 15.9 mm or 31.8 mm of structo-guard insulation, and exposed on its insulated face to the UL 1709 fire temperature curve. The skins are 6.4 mm thick, and the core is 76.2 mm thick. The bulkhead panel is 3.0 m in length.

The temperatures are predicted via the thermal model described in Chapter 3, and then fed into the thermal deflection model. The resulting maximum thermal deflection values as a function of time are provided in Figure 6.4.

Note that this model accounts for variable temperature, elastic modulus, and coefficient of thermal expansion profiles. These profiles are arbitrary, and thus may take into account the behavior of multiple panel layers (i.e. a sandwich panel in the current application). Furthermore, the panel does not directly require discretization to solve the problem. As such, the predicted thermal deflections may in fact be more accurate than those resulting from a coarsely discretized finite element approximation. The method does require the approximate numerical integration of the integrals defined in Equations (6.14), however. This integration is performed using the MATLAB `quad` function.

The lower limit on the fraction of undegraded elastic modulus mentioned in
Figure 6.4: Predicted maximum out-of-plane thermal deflections. The panel is a typical bulkhead CFRP/end-grain balsa cored sandwich panel. It is exposed to the UL 1709 fire temperature curve, with 15.9 mm insulation (left), and 31.8 mm insulation (right). The minimum property fraction will be described in more detail in Chapter 8.

Figure 6.4 turns out to be a key unknown with a significant impact on the accuracy of this whole methodology for predicting structural behavior. As such, the significantly differing results depicted in Figure 6.4, that depend upon this minimum property fraction so strongly, present an opportunity for this model to be used in conjunction with an experimental scheme to determine more accurately the mechanical properties of severely degraded FRP composite materials.

6.6 Conclusions

A model has been developed that accurately predicts the thermal deflections that are likely to result from the temperature profiles predicted by the thermal model. This model fully accounts for an arbitrary thermal profile, as well as for an arbitrarily-varying elastic modulus. An elasticity solution for the temperature-dependent coefficient of thermal expansion of the composite has been developed. The model also allows for the resulting arbitrarily-varying coefficient of thermal expansion profile to be accounted for. The model has been implemented numerically in a MATLAB code. An example application of the model is provided. This process offers a way to experimentally determine the mechanical properties.
of severely-degraded FRP composite materials.
Chapter 7

Material model

7.1 Introduction

In this chapter, a constitutive model is developed for FRP composite materials that inherently exhibits material level failure modes such as plastic microbuckling and shear induced kinking, in addition to larger-scale failure modes such as Euler macrobuckling; and in sandwich panels, shear induced macrobuckling and skin wrinkling [6]. The model is fundamentally different than those that are presently used to forecast the response of thermally degraded materials. For example, the two layer models of Gibson, Mouritz et al. [28, 65] are meant to describe the response of composite materials that have been severely degraded and that have experienced significant amounts of material loss through pyrolysis and char formation. The goal of this effort is to describe the response of materials that suffer a continuous range of degradation, including that occurring in non-charred material.

This model is formulated in such a manner that the effect of elevated temperatures on the material can be readily imposed. This constitutive model has been implemented in a finite element code. Structural models utilizing this material model may be set up, with degraded material properties resulting from the predictions of temperature profiles obtained from the thermal model and from property degradation curves, as determined from experimental measurements of material behavior at elevated temperature. The resulting models of fire-damaged structures, given a fire exposure, are able to describe the mechanical response;
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i.e. specify failure loads, failure times under given loads, and describe the failure modes that evolve and combine to produce overall failure.

7.2 Mechanical model

The ultimate goal for this aspect of the overall effort is a material model which describes both the mechanical response due to ablation (material loss) as well as the degradation in properties of the intact material. Material ablation will not be discussed herein. In the current work a theory describing time and temperature dependent elastic-plastic material response is described. This new theory is based in many aspects on the theory for crystal plasticity, especially as laid out by [7, 2], and [34]. This theory accounts fully for the anisotropy of FRP laminate elastic behavior as well as for the highly anisotropic inelastic response that occurs due to interlaminar shear, which is strongly influenced by temperature. The theory is developed herein—a complete development is available in [6].

Of particular interest is the ability of the model to describe common failure mechanisms that occur in compressively loaded FRP materials at elevated temperatures. In addition to global buckling modes such as Euler buckling and shear induced macrobuckling, as well as skin wrinkling in sandwich panels, we wish to describe plastic micro-buckling or kinking, which typically lead to rapid, often localized, degradation and fracture. We desire, therefore, a theory that naturally contains the occurrence of such phenomena as has been explored in simpler geometric models such as those given by Fleck et al. [13, 22]. The model need also contain an accurate description of the temperature dependence of material stiffness and material resistance to interlaminar shear as described in Chapter 8—these are accordingly key focuses of the development.

7.2.1 Nomenclature & conventions

Standard notations are used throughout. Bold-faced symbols are used to denote vectors and higher order tensors, the order of which will be clear in context. Products are indicated with dots, which denote summation over repeated Latin
indices, and products without dots are dyadic products. Latin indices range from one to the number of spatial dimensions (usually three), and repeated Latin indices are always summed. Inverses, transposes, and transpose inverses are denoted with a superscripted $-1$, $T$, and $-T$, respectively, and superposed dots indicate differentiation with respect to time, $t$. Greek indices are slip system identifiers ranging from one to two for the case of an orthotropic laminate such as considered herein and as explained below.

### 7.2.2 The laminate model

The FRP material is considered to be composed of an essentially orthotropic laminate, and to contain a sufficient number of plies so that homogenization is a reasonable way to describe the material behavior. The principal directions of the fibers are described by a set of mutually orthogonal unit base vectors, $\mathbf{a}$, as depicted in Fig. 7.1. The resulting orthotropic elastic response of the laminated composite will, thus, be fixed on, and described by these vectors. The material can also deform via slipping in the plane of the laminate, i.e. via interlaminar shear, and this slipping is confined to this interlaminar plane.

Two slip systems aligned with the slip directions $\mathbf{s}_1$ and $\mathbf{s}_2$ are introduced. The normal to the laminate plane is $\mathbf{m}$, and clearly $\mathbf{s}_1 \cdot \mathbf{m} = 0$ and likewise $\mathbf{s}_2 \cdot \mathbf{m} = 0$. It may well be natural, but not necessary, to take $\mathbf{s}_1$ and $\mathbf{s}_2$ to be orthogonal, i.e. $\mathbf{s}_1 \cdot \mathbf{s}_2 = 0$, but note that due to elastic distortions they may not remain so during deformation. These vectors will be called $\mathbf{s}_1^*$, $\mathbf{s}_2^*$, and $\mathbf{m}^*$ in the deformed state, but since $\mathbf{m}^*$ is to be the normal to the slip plane, i.e. the plane of the laminate, it will always be the case that $\mathbf{s}_1^* \cdot \mathbf{m}^* = 0$ and $\mathbf{s}_2^* \cdot \mathbf{m}^* = 0$ as shown to be naturally described by our expressions for the kinematics of laminate deformation.

In fact, it is possible to take the slip system vectors to be coincident with the laminate base vectors, $\mathbf{a}$, and insure that they are convected so that the above stated orthogonality is preserved; there is no need to do this however. Even though both slip systems have the same slip plane normal, i.e. $\mathbf{m}$, it will be convenient for symmetry of expression to refer to $\mathbf{m}_1$ and $\mathbf{m}_2$ in the expressions below. This makes it easier to establish correlations with the body of theory for crystal plasticity.
Figure 7.1: Kinematics of deformation. Note, the total deformation as prescribed by \( \mathbf{F} \) is decomposed into a process of interlaminar shear followed by an elastic deformation of the orthotropic framework. Thus \( \mathbf{F}^p \) describes the process of slip, or shear, across the laminate planes, a process whose kinematics are dictated by the local orientation of the laminate plane. Rigid body rotations, and elastic deformation, are described in \( \mathbf{F}^* \), the deformation gradient of the framework. It is upon this framework that elastic constants are constructed, in fact, in standard laminate models of elasticity [47].

This picture for viscoplastic deformation quite naturally describes the kinematics of shearing across a laminate as is, for example, specifically embodied in the models for shear induced kinking presented by Fleck et al. [13, 22], and earlier by Argon [1] (these authors build models that strictly fix plastic shearing across the laminate planes via simple shears). Figure 7.1 illustrates the total deformation from the reference configuration, \( \mathcal{B}_0 \), to occur in two stages producing a viscoplastic and an elastic deformation, respectively. The viscoplastic deformation occurs by the flow of the material through the framework, i.e. the lattice, of the laminate via the interlaminar shears. The spatial velocity gradient of this plastic flow is thus written as

\[
\dot{\mathbf{F}}^p \cdot \mathbf{F}^p^{-1} = \sum_{\alpha=1}^{2} \gamma_\alpha \mathbf{s}_\alpha \mathbf{m}_\alpha,
\]

where \( \mathbf{F}^p \) is the plastic deformation gradient and \( \gamma_\alpha \) is the rate of shearing on the
\( \alpha_{th} \) slip system. The value of \( F^p \) is obtained by the path dependent integration of (7.1). This process produces an intermediate configuration, \( B_p \). Next the current, i.e. deformed, configuration \( B_c \) is reached from \( B_p \) by elastically distorting and rigidly rotating the laminate (i.e. lattice) along with material, i.e. fabric and matrix, embedded on it. This second step of deformation is described by the elastic deformation gradient, \( F^* \). Hence the decomposition of \( F \),

\[
F = F^* \cdot F^p
\]  

(7.2)

is obtained, where \( F \) is the total elastic plus plastic deformation. This decomposition was introduced in this context for crystal plasticity by [7] and for phenomenological plasticity by [52].

The driving force for slip on the \( \alpha_{th} \) system is taken to be primarily the resolved shear stress, \( \tau_\alpha \) on that system. This is written as,

\[
\tau_\alpha = m^*_\alpha \cdot \tau \cdot s^*_\alpha,
\]

\[
s^*_\alpha = F^* \cdot s_\alpha,
\]

\[
m^*_\alpha = m_\alpha \cdot F^{*-1},
\]

\( \tau = J \sigma, \) 

(7.3)

where \( J = \text{det}\{F\} \) is the Jacobian, \( \tau \) is the Kirchhoff stress, and \( \sigma \) is the Cauchy stress (i.e. true stress). Here, in the current state (i.e. deformed state), \( s^*_\alpha \) and \( m^*_\alpha \) are respectively along the \( \alpha_{th} \) slip direction and the slip plane normal. Note that \( s_1 \) and \( s_2 \) are made to convect with the lattice framework whereas \( m \) is the reciprocal base vector that remains normal to the plane that contains both \( s_1 \) and \( s_2 \). This definition of \( \tau_\alpha \) as discussed by [3] is used because it makes \( \tau_\alpha \) conjugate to \( \dot{\gamma}_\alpha \), i.e. \( \sum_{\alpha=1}^{2} \tau_\alpha \dot{\gamma}_\alpha \) is precisely the plastic dissipation rate per unit reference volume.

On the other hand it is entirely possible that the shear resistance of interlaminar zones is sensitive to the normal stress that acts on the plane, the shear rate would depend on the stress component, \( \tau_{mm} = m^* \cdot \tau \cdot m^* \). In this case a more general load parameter might be prescribed for the \( \alpha_{th} \) slip system, viz. \( \hat{\tau}_\alpha = \|\tau_\alpha\| + \beta \tau_{mm} \), but where \( \hat{\tau} \geq 0 \). The parameter \( \beta \) represents frictional resistance due to the compaction of fabric resulting from normal compressive stresses. Note that as shown by [7] and then again by [18] the appearance of such terms in the loading parameter represents a deviation from the law of normality which, in turn, has implications for localized deformation.
The constitutive description of the plasticity on each slip system is cast in terms of the resolved shear stress on that system and on the current slip rate on that system as,

\[
\dot{\gamma}_\alpha = \dot{\gamma}_0 \text{sgn}\{\tau_\alpha\} \left\{ \frac{\|\tau_\alpha\|}{g_\alpha} \right\}^{1/m},
\]

where \(\tau_\alpha\) is the current value of the resolved shear stress and \(g_\alpha\) is the current value of the slip system hardness, i.e. the resistance to shear. In (7.4), \(m\) is the strain rate sensitivity exponent, \(\dot{\gamma}_0\) is a reference shear strain rate, and \(\text{sgn}\{\bullet\}\) means the sign of \{\bullet\}. Note that as \(m \to 0\) rate independent behavior is achieved, and that in that limit \(g_\alpha\) corresponds to the slip system strength, \(\tau_\alpha\), at least in absolute value. This limit is unlikely for the polymer resin systems of interest here. Also, for creep-like behavior we expect \(0 < m < 1\), whereas for viscoplastic response \(m \leq 0.1\).

In general, we expect that there may be hardening of the interlaminar layers following slip and this is described by a path dependent evolution equation of the form,

\[
\dot{g}_\alpha = \sum_{\beta=1}^{2} h_{\alpha\beta}(\gamma_a) \|\dot{\gamma}_\beta\|, \quad \gamma_a = \int_0^t \sum_\alpha \|\dot{\gamma}_\alpha\| dt,
\]

where \(h_{\alpha\beta}\) is a hardening matrix of (non-negative) hardening moduli and \(\gamma_a\) is the accumulated sum of the slips. The initial conditions for this evolution are specified as \(g_a(\gamma_a = 0) = g_0\) and the form of \(h_{\alpha\beta}\) is,

\[
h_{\alpha\beta}(\gamma_a) = g_t(\gamma_a) q_{a\beta},
\]

where the prime denotes differentiation with respect to \(\gamma_a\), and \(q_{a\beta}\) is a matrix that describes the cross hardening between the two slipping directions. A possible, and quite general form for \(g(\gamma_a)\) is,

\[
g(\gamma_a) = g_0 + h_\infty \gamma_a + (g_\infty - g_0) \tanh \left\{ \frac{\|\gamma_a\| (h_0 - h_\infty)}{g_\infty - g_0} \right\}.
\]

If the laminate is subjected to a monotonically increasing shear strain \(\gamma > 0\) along one direction, then \(\gamma = \gamma_a\) and the relation \(g = g(\gamma_a)\) can be interpreted as being the relation of hardness vs. shear strain for that slip system. Also, in (7.7), \(g_0 = g(\gamma_a = 0)\), \(h_0 = g_t(\gamma_a = 0)\), and \(h_\infty = g_t(\gamma_a \to \infty)\). If \(h_\infty \equiv 0\),
then $g_\infty = g(\gamma_a \to \infty)$. At present there is little data to guide the calibration of hardening laws such as (7.7), but its flexibility should provide the ability to do so.

The description of the laminate’s constitutive response is completed with a specification of its elasticity, which is expressed in terms of the Green strain of the fabric framework, viz. $E^* = (1/2)(F^{*T} \cdot F^* - I)$ and the laminate framework-based second Piola-Kirchhoff stress, $S^* = F^{-1} \cdot \tau \cdot F^{*-T}$, where $I$ is the second-order identity tensor. For anisotropic elastic solids the elastic response may be written as $S^*_{ij} = (\partial \Phi / \partial E^{*ij})$, where $S^* = S^*_{ij} a_i a_j$, $E^* = E^*_{ij} a_i a_j$, and $\Phi = \Phi(E^{*ij})$ is the free energy of the fabric framework per unit reference volume. Alternatively, in rate form, we have

$$\dot{S}^* = \mathbf{K} : \dot{E}^*, \quad \mathbf{K} = K_{ijkl} a_i a_j a_k a_l, \quad K_{ijkl} = \frac{\partial^2 \Phi}{\partial E^{*ij} \partial E^{*kl}}. \quad (7.8)$$

On the other hand $\mathbf{K}$ can, and typically will, be constructed from a laminate theory based on discrete analysis of the layering of thin plies.

### 7.2.3 Additional kinematical perspective

The decomposition of (7.2) results in the total velocity gradient taking the form,

$$\dot{F} \cdot F^{-1} = \dot{F}^* \cdot F^{*-1} + F^* \cdot \sum_{\alpha=1}^2 \dot{\gamma}_\alpha s_\alpha m_\alpha \cdot \dot{F}^{*-1}. \quad (7.9)$$

By forming symmetric and antisymmetric parts of the above velocity gradient we obtain the decomposition of the rate of deformation and the spin rates, viz.

$$\mathbf{D} = \mathbf{D}^* + \mathbf{D}^p \quad \Omega = \Omega^* + \Omega^p, \quad (7.10)$$

where

$$\mathbf{D}^p = \sum_{\alpha=1}^2 \mathbf{P}_\alpha \dot{\gamma}_\alpha \quad \Omega^p = \sum_{\alpha=1}^2 \mathbf{W}_\alpha \dot{\gamma}_\alpha. \quad (7.11)$$

In (7.11), the symmetric and antisymmetric tensors $\mathbf{P}_\alpha$ and $\mathbf{W}_\alpha$ are given as,

$$\mathbf{P}_\alpha = \frac{1}{2} \{s^*_\alpha m^*_\alpha + m^*_\alpha s^*_\alpha \} \quad \mathbf{W}_\alpha = \frac{1}{2} \{s^*_\alpha m^*_\alpha - m^*_\alpha s^*_\alpha \}. \quad (7.12)$$

The elastic parts of $\mathbf{D}$ and $\mathbf{W}$, viz. $\mathbf{D}^*$ and $\mathbf{W}^*$ are formed by taking the symmetric and antisymmetric parts of (7.9). Note that the interpretations of how $s$ and $m$
convect with the laminate framework, as introduced in (7.3), are a natural outcome of the kinematical scheme shown in Fig. 1.

7.2.4 Final constitutive forms

The description of the lamella constitutive response is completed with a specification of its elasticity, which is expressed in terms of the Green strain of the framework, $\mathbf{E}^*$, as given by $\mathbf{E}^* = \frac{1}{2} (\mathbf{F}^* \cdot \mathbf{F}^* - \mathbf{I})$. Having the description of this response the entire constitutive theory can be expressed in terms of the Green strain, $\mathbf{E} = 1/2(\mathbf{F}^T \cdot \mathbf{F} - \mathbf{I})$ and the second Piola-Kirchhoff stress, $\mathbf{S} = \mathbf{F}^{-1} \cdot \mathbf{\tau} \cdot \mathbf{F}^T$. Straightforward tensor manipulations of the above relations yield the governing constitutive rate form,

$$\dot{\mathbf{S}} = \mathbf{L} : \dot{\mathbf{E}} - \sum_{\alpha=1}^{2} \dot{\gamma}_\alpha \mathbf{X}_\alpha,$$  \hspace{1cm} (7.13)

where

$$L_{ijrn} = F_{ik}^{p-1} F_{jt}^{p-1} K_{klpq} F_{rp}^{p-1} F_{nq}^{p-1}.$$  \hspace{1cm} (7.14)

and where

$$\mathbf{L} = L_{ijkl} a_i a_j a_k a_l, \quad \mathbf{F}^{p-1} = F_{ij}^{p-1} a_i a_j.$$  \hspace{1cm} (7.15)

In (7.13)

$$\mathbf{X}_\alpha = \mathbf{F}^{p-1} \cdot \{ \mathbf{K} : \mathbf{A}_\alpha + 2\mathbf{B}_\alpha \} \cdot \mathbf{F}^{p-1},$$  \hspace{1cm} (7.16)

with

$$\mathbf{A}_\alpha = \text{sym} \{ \mathbf{F}^{*T} \cdot \mathbf{F}^* \cdot \mathbf{s}_\alpha \mathbf{m}_\alpha \}, \quad \mathbf{B}_\alpha = \text{sym} \{ \mathbf{s}_\alpha \mathbf{m}_\alpha \cdot \mathbf{S}^* \}.$$  \hspace{1cm} (7.17)

Finally, we note that it is useful to express the constitutive relations in terms of the nominal stress, $\mathbf{n}$ and its conjugate, $\mathbf{F}$ itself. The transformation is also straightforward since $\mathbf{n} = \mathbf{F}^{-1} \cdot \mathbf{\tau} = \mathbf{S} \cdot \mathbf{F}^T$ and consequently $\dot{\mathbf{n}} = \dot{\mathbf{S}} \cdot \mathbf{F}^T + \mathbf{S} \cdot \dot{\mathbf{F}}^T$, which then yields

$$\dot{\mathbf{n}} = \mathbf{M} : \dot{\mathbf{F}} - \sum_{\alpha=1}^{2} \dot{\gamma}_\alpha \mathbf{Y}_\alpha,$$  \hspace{1cm} (7.18)
with

$$M_{ijkl} = F_{ia}^{p-1}F_{jd}^*K_{abcd}F_{kc}^{p-1}F_{id}^* + S_{ik}\delta_{jl} \quad (7.19)$$

$$\mathbf{F}^* = F_{ij}^*a_i a_j, \quad \mathbf{S} = S_{ij}a_i a_j \quad (7.20)$$

$$\mathbf{I} = \delta_{ij}a_i a_j, \quad \mathbf{M} = M_{ijkl}a_i a_j a_k a_l. \quad (7.21)$$

with

$$\mathbf{Y}_\alpha = \mathbf{X}_\alpha \cdot \mathbf{F}^T. \quad (7.22)$$

### 7.2.5 Calibration of the constitutive model

To account for the loss in material stiffness at elevated temperatures we will take, as a first step, a degradation curve that will be shown subsequently in Figure 8.3 to be a master degradation function for all components of moduli. This means that in (7.8) and (7.14) $K_{ijkl} \leftarrow f(T)K_{ijkl}$, where $f(T)$ is the monotonically decreasing function shown in that figure. It should be possible to improve on this simple representation of stiffness degradation with further experimental study of the effect of temperature on anisotropic stiffness. Losses in shear strength are handled, again as a first step in our modelling, by replacing $g(\gamma_a)$ in (7.4) with $\eta(\gamma_a)$, where $\eta = r(T)g(\gamma_a)$. The function $r(T)$ is the linearly decreasing function that will be shown subsequently as the second curve in Figure 8.4. Thus, the shearing rates are calculated from,

$$\dot{\gamma}_\alpha = \dot{\gamma}_\alpha sgn\{\tau_\alpha\} \left\{\left[\frac{\tau_\alpha}{\eta_\alpha}\right]\right\}^{1/m}. \quad (7.23)$$

In general, orthotropic elastic symmetry is presumed although the materials will often possess transverse isotropy. Thus the elastic constants will have components, when phrased on the orthotropic axes of the form,

$$\mathbf{K} = K_{ijkl}a_i a_j a_k a_l. \quad (7.24)$$

If the common convention of index contraction is used, i.e. $11 \rightleftharpoons 1, 22 \rightleftharpoons 2, 33 \rightleftharpoons 3,$
23, 32 = 4, 13, 31 = 5, and 12, 21 = 6, the matrix of components becomes,

\[ K = \begin{pmatrix}
  K_{11} & K_{12} & K_{13} & 0 & 0 & 0 \\
  K_{12} & K_{22} & K_{23} & 0 & 0 & 0 \\
  K_{13} & K_{23} & K_{33} & 0 & 0 & 0 \\
  0 & 0 & 0 & K_{44} & 0 & 0 \\
  0 & 0 & 0 & 0 & K_{55} & 0 \\
  0 & 0 & 0 & 0 & 0 & K_{66}
\end{pmatrix} \]  

(7.25)

the elements of this stiffness matrix may be formed directly from experimental measurement of the elastic moduli, or from standard laminate theory. We note, however, that for our simulation to be described isotropic, elastic behavior is assumed.

### 7.2.6 Kinking of sandwich composite skin

The constitutive model just described has been implemented in a finite element model to demonstrate its ability to represent the occurrence of kinking, in addition to other failure modes. Here we briefly describe one such simulation for the purpose of demonstrating and explaining this feature of the model. While we are herein purposely focusing on describing a material failure mode, it must be emphasized that the theory fully accounts for all larger scale structural deformation and failure modes. These include, of course, overall structural deformation and failure due to collapse caused by buckling. We note, as discussed above, that with degradation due to elevated temperatures; interlaminar shear, i.e. slip, is induced and this will lead to an early onset of failure modes such as kinking. Of course, other failure modes such as skin wrinkling are also likely to be triggered and these will compete with failure modes such as structural buckling and kinking.

A sandwich panel was modelled, with a relatively “stubby” aspect ratio to preclude the occurrence of Euler buckling or other failure modes before the formation of a kink band. The sandwich was taken to be symmetric and consisted of a relatively compliant core and skins of symmetric lay-up with respect to the mid-plane of the sandwich. The skins were joined to the core via an adhesive layer, which
was allowed to debond. The constitutive model outlined above was used for the composite skin with slip plane normal parallel in the reference configuration to the surface of the skin. A geometrical imperfection in the slip plane normal at about the midpoint of the panel, i.e. between \( z = 35 \) mm and \( z = 45 \) mm (the panel is 100 mm in height), the direction of the normal is assumed to have components \( \tilde{N}_x = 1 \) (horizontal in Figure 7.2), \( \tilde{N}_y = 0 \) (normal to cross section shown in Figure 7.2), and

\[
\tilde{N}_z = -\frac{\pi}{20} \sin \left( \frac{\pi}{10} (z - 35) \right)
\]

(7.26) (vertical in Figure 7.2). The actual slip plane normal is normalized to unit length, \( N_i = \tilde{N}_i/||\tilde{N}|| \).

Figure 7.2 shows the evolution of the plastic slip strain \( \gamma_2 \) during kink formation, that is, the development of the inelastic deformation. The possibility of the

Figure 7.2: Distribution of the shear strain \( \gamma_2 \) at the imperfection area in the deformed specimen. The range of the color map of the contours is fixed at \(-0.05 \leq \gamma_2 \leq 0.05\). The displacement in the transverse direction has been magnified by 10 for clarity.

formation of such a plastic kink band is thus clearly demonstrated to result from the use of this constitutive framework.

We again note that the purpose of this example is to explain how this model naturally describes such material level phenomena. In typical scenarios involving structural members, failure may be initiated via global buckling, which may then be followed by such material level failure modes. The precise sequence of all such failure modes, as well as their interactions, can therefore only be described by a theory that naturally contains all such modes.
7.3 Summary and future work

In this chapter a material model has been detailed which inherently accounts for such material-level failure modes as shear kinking or plastic microbuckling, in addition to Euler buckling, shear macrobuckling and skin wrinkling. Key material properties in this model may be degraded per the temperature predictions provided by the thermal model discussed in Chapter 3, used with the degradation relations to be provided in Chapter 8, to account for the mechanical effect of the elevated temperatures. This model, used in this way, can predict the response of an arbitrary structure exposed to fire, i.e. to determine failure loads, failure time under given loads, and failure type.

Finally it is noted that including a description of viscoelastic response in this material model is entirely straightforward given its physically-based structure. For example, in-plane viscoelastic deformation would be described by shearing along fiber directions and across planes lying normal to the laminate plane. These effects are currently being included. They will be more fully assessed as experimental data that specifically includes the measurement of evolving strain to loading and unloading, as well as variable load vs. time histories, becomes more generally available.

7.4 Acknowledgements

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Chapter 8

Material model properties and degradation relations

8.1 Introduction

In this section material properties for use in the material model developed in Chapter 7 are determined. These include the elastic constants used to describe the elastic portion of the mechanical behavior. Also included are the constants which determine the plastic portion of the mechanical behavior. The thermal degradation relation for the elastic constants must then be determined. Finally, the thermal degradation relation for select shear-driven plasticity constants will be determined.

8.2 Mechanical properties

8.2.1 Elastic behavior

The elastic constants which describe the elastic portion of the deformation (as shown in Figure 7.1) must first be described. The elastic constants required by the model are the unique elements of the stiffness matrix given in Equation (7.25); i.e. $C_{11}$, $C_{12}$, and $C_{44}$. Values for these constants will be determined indirectly via the modulus of elasticity $E$ and Poisson’s ratio $\nu$, however.

For the modulus of elasticity $E$, a value for a woven glass/vinylester composite
of 17.7 GPa is available from Mouritz et al. [65]. The composite of interest for the current application is a quadraxial glass/vinylester composite. To estimate the value for the quadraxial material, the value for the woven material is multiplied by a factor of 0.9 (the ratio for quadraxial to woven for carbon/epoxy composites in the same paper). This yields an estimated modulus for quadraxial eglass/vinylester of 15.8 GPa.

For the Poisson’s ratio of the composite, a value for the material of interest was unavailable, and so a value of 0.37 given for a carbon/epoxy composite is used [16]. These values result in Lamé constants (assuming elasticity) of $\lambda = 16.9$ GPa and $\mu = 5.75$ GPa. Finally, the unique elastic constants are given as $C_{11} = 28.4$ GPa, $C_{12} = 16.9$ GPa, and $C_{44} = 5.75$ GPa.

Mechanical properties for various core materials are available in the product literature [20]; for balsa wood in particular a Poisson’s ratio of 0.0 is assumed, to yield a value for the shear modulus comparable to that given in [11]. Elastic moduli for the radial and tangential directions for balsa wood are also available per [11].

### 8.2.2 Inelastic behavior

Various parameters must be determined to characterize the plastic behavior of the composite laminate. These include the reference shear strain rate $\dot{\gamma}_0$, the initial flow stress $g_0$, the saturation flow stress $g_\infty$, the initial hardening modulus $h_0$, and the strain-rate sensitivity exponent $m_{\text{rs}}$. The initial flow stress $g_0$, the saturation flow stress $g_\infty$, and the initial hardening rate $h_0$ are needed to determine the current flow stress as a function of the accumulated shear strain in the general hardening model presented in Equation (7.7). The reference shear strain rate $\dot{\gamma}_0$ and the strain-rate sensitivity exponent $m_{\text{rs}}$, together with the current flow stress from the hardening model, are used to determine the current slip rate in each slip system according to Equation (7.4).

To estimate values for these parameters, experimental data available from research conducted by Scott Case et al. at Virginia Tech are utilized. These data provide the creep response of an E-glass/vinylester composite. In particular, a bi-
axial laminate was loaded in tension at a 45° angle to both laminate directions. The stress (i.e. load) was held constant, and the time-dependent strain was recorded. This process was repeated at various temperatures and stress (i.e. load) levels.

To determine the needed parameters, the time-dependent strain records for six stress levels at constant temperature; in particular 100, 200, 500, 1000, 1500, and 2000 psi, each at 90°C; were examined. This data is plotted in Figure 8.1.

![Normalized strain vs. time, temp. = 90°C](image)

Figure 8.1: Experimentally measured normalized strain as a function of time at various loads and at a constant temperature of 90°C, log/log plot.

An implementation of the material model provided in Chapter 7 at a single Gauss point was used to duplicate this behavior. The goal was to optimize the fit for all six of these curves simultaneously. The MATLAB `fminsearch` implementation of the Nelder–Mead simplex algorithm was utilized for this purpose. This algorithm performs an unconstrained optimization, perhaps resulting in optimal values that are not physically reasonable. To restrict the search to within reasonable bounds for each parameter, penalty functions were used. The general penalty function format is provided in Equation (8.1).

\[ p = \max\left(0, \frac{p_{\text{incr}}}{x_{\text{incr}}} \cdot (x - x_{\text{lim}})\right) \]  

(8.1)

In Equation (8.1), \( x \) is the current parameter value, \( x_{\text{lim}} \) is the limiting parameter
Table 8.1: Penalty functions for use in unconstrained optimization to find mechanical plasticity parameter values.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Limit type</th>
<th>$x_{lim}$</th>
<th>$x_{incr}$</th>
<th>$p_{incr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma_0$</td>
<td>lower</td>
<td>$1 \times 10^{-12}$</td>
<td>$-1 \times 10^{-12}$</td>
<td>1</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>upper</td>
<td>$1 \times 10^{-3}$</td>
<td>$1 \times 10^{-3}$</td>
<td>1</td>
</tr>
<tr>
<td>$g_0$</td>
<td>lower</td>
<td>0.001</td>
<td>-0.001</td>
<td>1</td>
</tr>
<tr>
<td>$g_0$</td>
<td>upper</td>
<td>$g_\infty - 0.01$</td>
<td>0.01</td>
<td>1</td>
</tr>
<tr>
<td>$g_\infty$</td>
<td>lower</td>
<td>$g_0 + 0.01$</td>
<td>-0.01</td>
<td>1</td>
</tr>
<tr>
<td>$h_0$</td>
<td>lower</td>
<td>0.01</td>
<td>-0.01</td>
<td>1</td>
</tr>
</tbody>
</table>

value, $x_{incr}$ is some incremental distance beyond the parameter value, and $p_{incr}$ is the penalty to be applied at distance $x_{incr}$ from $x_{lim}$. Note that if the limiting value is to be a minimum limit on the parameter, $x_{incr}$ should be negative, while if the limiting value is to be a maximum limit, $x_{incr}$ should be positive. The penalty functions specified are provided in Table 8.1.

The score to minimize was given by the equation

$$S = \frac{\|\gamma_{model} - \gamma_{exper}\|_2}{\|\gamma_{exper} - \gamma_{exper}(t = t_0)\|_2}$$

(8.2)

where the denominator is used to ensure that each of the curves receives about the same weighting, whereas without this normalization, the higher curves (with higher numerical values) would dominate the scoring.

This function was found to have numerous local minima. To best determine a global minimum, the search was performed using a grid of 108 initial parameter value combinations; in practice, however, only 97 of these combinations were run. The combinations included all combinations of the values given in Table 8.2 except for all combinations containing $\gamma_0 = 1 \times 10^{-10}$, $g_0 = 0.25$, and $g_\infty = 20$ or 6; excluding the combination with $g_\infty = 20$, $h_0 = 10000$, and $m_{srs} = 0.02$, which was run. These combinations were deemed to be unlikely to lead to an optimal result, and thus were not run to save time.

The resulting optimum values for the parameters are reference shear strain rate $\gamma_0 = 1.815 \times 10^{-6}$, initial hardness $g_0 = 0.0386$ MPa, final hardness $g_\infty = 6.63$ MPa, hardness modulus $h_0 = 6950$, and strain rate sensitivity exponent $m_{srs} = 0.0727$. The optimum fit is shown in Figure 8.2. Note that the fit, while satisfactory, is
Table 8.2: Initial values used in optimization search to determine mechanical plasticity parameter values.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$x_{0.1}$</th>
<th>$x_{0.2}$</th>
<th>$x_{0.3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma_0$</td>
<td>$1 \times 10^{-6}$</td>
<td>$1 \times 10^{-10}$</td>
<td></td>
</tr>
<tr>
<td>$g_0$</td>
<td>0.05</td>
<td>0.1</td>
<td>0.25</td>
</tr>
<tr>
<td>$g_\infty$</td>
<td>50</td>
<td>20</td>
<td>6</td>
</tr>
<tr>
<td>$h_0$</td>
<td>10000</td>
<td>100</td>
<td></td>
</tr>
<tr>
<td>$m_{srs}$</td>
<td>0.02</td>
<td>0.2</td>
<td>0.75</td>
</tr>
</tbody>
</table>

Figure 8.2: Optimized fit of model to experimentally measured normalized strain as a function of time at various loads and at a constant temperature of 90 °C, log/log plot.

less than ideal—this is due not to a failure of the optimization algorithm, however, but due to the lack of suitability of the hardening model.
8.3 Thermal degradation of mechanical properties

8.3.1 Thermal degradation of elastic constants

The elastic constants in Equation (7.25) are to be degraded to account for the loss of stiffness resulting from the glass transition in the matrix resin. Measured data yield the following degradation relations, as plotted in Figure 8.3:

For FRP composites, the elastic constants are to be degraded according to the relation

\[
\frac{X}{X_0} = 307 - 46.0T + 0.276T^2 - 0.000823T^3 + 1.229 \times 10^{-6}T^4 - 7.33 \times 10^{-10}T^5 \quad (8.3)
\]

Note that for this degradation relation (and for all others given in this chapter), the temperature \(T\) is given in Kelvin, and the expression is subject to the following condition:

\[
\frac{X}{X_0} = \max \left( \min \left( \frac{X}{X_0}, 1 \right), \frac{X}{X_{0\min}} \right) \quad (8.4)
\]

Thus values are limited to being less than or equal to unity and greater than or equal to a minimum fraction value. This minimum fraction value is an arbitrary small non-zero number that serves only to ensure that completely degraded elements do not have zero stiffness.

Figure 8.3: Degradation of elastic constants with temperature.
A degradation relation for balsa wood is also available, and is given by

\[ \frac{X}{X_0} = -2.41 + 0.0234 T - 0.00004 T^2 \]  

(8.5)

A degradation relation for structural foam is likewise available, and is given by

\[ \frac{X}{X_0} = -3.49 + 0.0328 T - 0.000596 T^2 \]  

(8.6)

8.3.2 Degradation of shear constants

The next step is to determine the thermal degradation of the shear properties—namely the initial hardness, the final hardness, and the hardness modulus. To estimate this, optimum values for these parameters were determined for multiple temperatures (30°C, 60°C, 90°C, and 110°C) but at constant stress level. This then yields four average property fractions, one corresponding to each temperature value. The undegraded property fraction is not known, but is estimated such that the fitted curve lines up well with the optimized values. The expression plotted is

\[ \frac{X}{X_0} = 3.31 - 0.00787 T \]  

(8.7)

where \( T \) is the temperature in Kelvin.

Figure 8.4: Degradation of shear properties with temperature.
8.4 Conclusion

In this chapter material properties for use in the material model have been determined. As well, degradation relations for key properties with temperature have been provided.

It is important to note that the degradation relation for the mechanical properties of FRP composites given in Equation (8.3), though conservative, is less than ideal. In particular, even after passing beyond the glass transition temperature, the composite still maintains a significant fraction of its initial property value. This fraction will increase with thicker composites, as even after the resin has lost its stiffness, the fibers will still remain in place to some extent. Thus the use of this degradation relation should lead to conservative design estimates, though it should be understood to be overly conservative when used to predict experimental behavior.
Chapter 9

Structural modelling

9.1 Introduction

In this section, the creation of structural finite element models, implementing the material model and using degraded mechanical properties, is described. These models are created in such a way as to enable the possible occurrence of all relevant failure modes.

In practice, this process is carried out by first running the thermal model (as described in Chapter 3), and having it write the temperature prediction with time to an output file, together with a description of the spatial discretization used therein.

A separate program, from here on referred to as cif s, short for “create input file script,” is then run to generate the degraded finite element models. This program reads in the thermal model output file. It requires the description of the mesh geometry, of the material properties, of the boundary conditions, and of the dynamic solution control parameters.

This program, using the defined parameters, creates the mesh geometry. It then interpolates the temperature values at given times at the element midpoints for the defined structural geometry. These temperatures are then passed into the relevant degradation functions to yield two arrays, one of degraded elastic constant fractions at specified times, and another of degraded shear constant fractions at these specified times.
This data is then used to create an input file for the WASP finite element code developed by Professor Petr Krysl. For this another function is run, which from here on will be referred to as cif, short for “create input file.” This secondary program writes out in the newly created input file the mesh geometry (nodes and elements), the material definitions, the load and displacement boundary conditions, etc.

The WASP program has available implicit and explicit solvers. A quasi-static solver was not available. As the convergence of the implicit solver was poor, the explicit solver was utilized, and the problem was solved via dynamic relaxation.

A separate input file is therefore created for each “snapshot” in time at which the stable configuration of the degraded panel (i.e. the configuration of the panel at that instant in time) is to be determined. A script is automatically generated, which runs each input file one-by-one. Thus only one command need be issued to run all finite element models (one full model for each time instant).

Failure of one of these models indicates that the structure failed at or before that time instant, and the mode of failure at times at or near the failure time can be observed directly.

In the following sections, this process is described in more detail, with particular attention paid to the creation of the structural models.

9.2 Required information

The cif program requires several parameters to be defined. These parameters will be described in this section.

9.2.1 Mesh geometry

The cif program requires that the mesh geometry be specified. This includes the panel geometry (i.e. the panel length, width, skin thicknesses, core thickness, debonding layer thickness, etc.). When panels may be represented as plane strain, the width and debonding layer thickness (if required) are assigned as the minimum core or skin element dimension—thus these dimensions do not reduce the critical
time step for the explicit solver. From the panel dimensions and the number of elements in each direction, the element dimensions are obtained directly.

Another two parameters which affect the mesh geometry and therefore must be specified for sandwich panels concern geometric imperfections which are to be imposed upon the skins to enable the occurrence of skin wrinkling. This involves displacing the nodes in the hot face or in both faces by a small amount in the shape of a sine wave in the $x$ coordinate (through-panel) direction.

In particular, two parameters must be specified, a wavelength $\lambda$ and a maximum angle with the vertical ($z$) direction, $\theta$. The amplitude of the sine wave is given in terms of $\lambda$ and $\theta$ as $\frac{\lambda}{2\pi} \tan(\theta)$.

Niu and Talreja provide an elasticity solution for the skin wrinkling problem. In particular, they provide, as Equation (20) in Reference [67], the critical skin wrinkling stress as a function of the material properties, the panel geometry, and $n$. Note that $\alpha_n = \frac{n\pi}{L}$, wherein $n$ is the number of waves along the panel length in a given wrinkling mode. Furthermore, note that the skin wrinkling wavelength $\lambda_0$ is given by $\lambda_0 = \frac{\pi}{\alpha_n} = \frac{L}{n}$. Thus to find the critical skin wrinkling wavelength, i.e. the wavelength at which the skin wrinkling stress is minimal, one must only find the wavelength that minimizes the stress given in Equation 20 in Reference [67]. This is performed numerically using the Newton/Raphson method, with the initial guess for the wavelength given for instance in Equation (6) in Reference [67].

### 9.2.2 Material properties

The material parameters must also be specified. For sandwich panels, these include (as discussed in Chapter 8) the elastic modulus and Poisson’s ratio of the core material, the debonding strength of the core material and skin/core adhesive (for use in the debonding layer).

Also required is the elastic modulus and Poisson’s ratio for the FRP composite. The Lamé constants are determined from these. Furthermore, the parameters which govern the interlaminar shear strain behavior as described in Chapter 8 are required, including the reference shear strain rate $\gamma_0$, the initial flow stress $g_0$, the saturation flow stress $g_\infty$, the initial hardness modulus $h_0$, and the strain-rate
In order to ensure the possible occurrence of plastic microbuckling, which is driven by the presence of an imperfection angle in the fibers, imperfection angles must be placed in the laminate materials. Quantification of such imperfection angles as measured in laminates is available in the literature. In particular, Yurgartis has found out-of-plane imperfection angles to have a standard deviation of $0.947^\circ$ [92]. Thus the out-of-plane mean imperfection angle is defined as zero, and the value from Yurgartis is used as the standard deviation. Finally, a number of imperfection angles parameter is specified. This defines a set number of imperfection angles ($n_{ias}$) which will be determined via sampling the defined normally-distributed probability distribution function (using Latin hypercube sampling) to get $n_{ias}$ imperfect materials for each composite layer in the hot skin.

9.2.3 Boundary conditions

The cifs program also requires the definition of the boundary conditions. In particular, any distributed in-plane loads and out-of-plane loads must be defined. As well, the loaded surfaces should be specified for the in-plane load (i.e. the hot skin, the core, and/or the cold skin at the panel ends). This is useful, as for sandwich panels in which the hot skin is substantially degraded, it may be desirable to apply the load to the core and cold face only, as these are more likely to bear the load.

A load ramping function must also be specified. The purpose of this will be discussed in more detail subsequently.

The displacement boundary conditions must also be specified. For instance, the out-of-plane ($x$) displacement is generally set to zero at the cold face at the top and bottom of the panel (allowing the ends to rotate). Also, for panels modelled as plane-strain, the $y$ displacement is restrained. Finally, the unloaded (bottom) end of the panel is either uniformly restrained in the $z$ direction (fixed) or thus restrained along one row of nodes (pinned).
9.2.4 Dynamic solution control parameters

A few parameters must be specified which govern the explicit solution in the WASP program. The time step at which to record displacements and other numerical data must be specified. This should be relatively small, and is used to view the dynamic relaxation process. As well, the time step at which to generate visual output files (which may be viewed on the postprocessor) needs to be specified. The only meaningful visual output file is that upon reaching stable equilibrium.

The target time must be specified, which in this case is a time before which the equilibrium state has been reached (i.e. the dynamic relaxation process has completed). As well, a Rayleigh mass-proportional damping coefficient need be specified. This coefficient is determined via trial and error such that the dynamic relaxation process proceeds most efficiently—i.e., is near-critical, or just under critical. It is not desired to have the system significantly overdamped or underdamped, as this will lead to the equilibrium state taking longer to be reached.

9.3 Procedures used

With all needed parameters specified, the cifs program utilizes several methods in the generation of the WASP input files that are of interest. These are briefly described herein.

9.3.1 Mesh creation

To generate the finite element mesh, or in other words the arrays of node and element definitions, several tasks must be accomplished. First, the node array must be generated, accounting for the panel geometry and spatial discretization as specified.

The second task is to create the elements array. For plane strain problems, eight node hexahedral elements with $2 \times 2 \times 2$ Gaussian quadrature are used. For other problems, twenty-node hexahedra are used. Twenty-node hexahedra cannot be utilized for plane strain problems as it is not possible to restrain the interior nodes to obey the plane-strain boundary condition—that is, they are free to bulge
out, or to displace relative to the adjacent end point nodes, when to satisfy the plane strain boundary condition they must not displace relative to the adjacent end point nodes.

Of particular interest is the assignment of the material identifier to degraded elements, to elements with random imperfection angles assigned to the material, and to elements matching both of these criteria. For degraded element layers within a given material, a single degraded material may be defined for each layer. For element layers within a material with varying imperfection angle, there will be $n_{i_{as}}$ materials defined per layer, each with a different imperfection angle, as selected via Latin hypercube sampling. Material identifiers are then randomly selected for each element in that layer from among the $n_{i_{as}}$ materials.

The slip plane normals are initially normal to the lamina plane; the slip directions are within the lamina plane and $\pm 45^\circ$ from vertical (i.e. the positive $z$ direction). To represent the slip plane imperfections, these vectors are transformed to account for the imperfection angle.

9.3.2 Node displacement for geometric imperfections

A function is used to displace nodes within specified windows (i.e. the hot face away from the panel ends) per the geometric imperfection parameters $\lambda$ and $\theta$ as previously defined.

9.3.3 Determine fractions of undegraded material properties

A function is used to determine, based upon the thermal model prediction (or temperatures measured experimentally), the degraded mechanical properties for each layer of elements in the structural model. This involves first determining the structural model element midpoint locations. The temperatures at the thermal model nodes and at the structural model times are then interpolated (using piece-wise cubic Hermite interpolation). Next the temperatures at the structural model element midpoints and at the structural element times are likewise determined.
Finally, these temperatures are passed into the relevant degradation functions (i.e. separate functions for skins and core, etc.).

## 9.4 Input file creation

A function to write out the input file is then called. This \texttt{cif} function creates the input file, and writes out within it the relevant headers and options. Next, time functions are defined. The load is not applied instantaneously in the dynamic simulation, but is ramped up linearly over time until the desired load is reached, and then this load is maintained.

Next the material definitions are written to the input file. In general, a few elements at the panel ends are left undegraded, so as to distribute applied loads and reaction forces. So the materials to be defined include the undegraded core, the undegraded debonding layer, the undegraded skin 1 and skin 2 materials, the degraded core, and the degraded debonding layer. For each degraded layer of composite, \( n_{\text{ias}} \) materials must be defined, where \( n_{\text{ias}} \) is the number of imperfection angles. A typical value used for \( n_{\text{ias}} \) is fifty. Thus, for a sandwich panel model with \( n_{s1} = 4, n_c = 4, n_{s2} = 2, \) and \( n_{\text{ias}} = 50; \) there would be 213 materials defined.

Next the node array and the element array are written to the input file. These were defined previously.

The loads are then written out, to be multiplied by a time function as already defined. The loads are applied at the nodes via lumping. The general process here is to first decide which nodes are to be loaded, and to store the node IDs of these loaded nodes in a vector. If multiple input files are to be generated, these vectors are stored, and do not have to be regenerated. For each loaded node, the lumped load fraction is then determined via the position relative to the panel edges. The loads are then written to the input file.

The displacement boundary conditions are then defined. These have been discussed previously. Finally, a list of nodes and element Gauss points at which to record history data is defined. Again, these node numbers are found via a search, and the node indexes are stored. In general, nodes along the center line of the
panel (in the hot skin and on the inside edge of any debonding layer), and at Gauss points in one set of elements adjacent to these nodes, are included. Also included is a node at the top of the panel at the inside face of the top skin. The nodes at the panel midpoint (along the panel length) will reveal the out-of-plane displacement. The node at the top of the panel will reveal the in-plane displacement. The element Gauss points in at the midpoint of the panel will show stress and plastic strains, if any plastic behavior is observed.

9.5 Dynamic solution

Initially models are run at various damping levels until the Rayleigh mass-proportional damping coefficient has been determined such that the damping is just under critical.

For the model behavior to be accurate, especially when the post-failure behavior is of interest, a quasistatic solution must be ensured (i.e. inertial effects must be kept minimal). This can be judged by for instance ensuring that the kinetic energy of the system remains small as a fraction of its total energy—i.e., this fraction is kept to less than 5% or so [39].

The loading is ramped up in some fashion from zero initially to the specified load after a given time. This time and ramping function are selected such that the loading is gradual enough that inertial effects do not become significant—thus the quasistatic response is observed even though the problem solution takes place at an accelerated time scale.

Mass scaling may be used to speed up the dynamic solution. The time step for the explicit solution is limited to

\[ \Delta t \leq \left( \frac{1}{L} \sqrt{\frac{\rho}{\lambda + 2\mu}} \right) \]  

where \( L \) is the element length, \( \rho \) the mass density, and \( \lambda \) and \( \mu \) are the Lamé constants. Thus by increasing the mass densities by a factor \( \rho_{\text{mult}} \), the time period of load application is reduced by a factor of \( 1/\sqrt{\rho_{\text{mult}}} \), but the time scale is preserved.

Thus the mass density is increased, and the loading time decreased, until the
kinetic energy exceeds 5% or so of the internal strain energy. This ensures that inertial effects do not become significant [39].

9.6 Example

Herein an example problem will be described. In particular, this is a typical bulkhead sandwich panel in a naval application. The panel is three meters in length. It has carbon fiber/vinylester skins, $t_{s1} = t_{s2} = 6.4$ mm; and an end-grain balsa core, $t_c = 76.2$ mm. It is insulated with one of two thicknesses of structoguard insulation, $t_{ins} = 15.9$ mm, or $t_{ins} = 31.8$ mm. It is exposed to the UL1709 fire temperature curve. It is in a pin/pin configuration, and loaded in compression, with either $P = 29.2$ N/mm, or $P = 43.8$ N/mm. The problem is plane strain. As such, eight node hexahedral solid elements are used.

The spatial discretization is as follows: $n_{s1} = 2$, $n_c = 3$, and $n_{s2} = 1$; $n_y = 1$, and $n_z = 300$. A debonding layer is added to the core, just inside the hot face. This material has the same properties as the core material, but loses its stiffness if the maximum principle stress exceeds a tensile cutoff stress. Thus there are two layers of degraded skin one material (with various imperfections), one layer of degraded core material capable of debonding, three layers of degraded core material incapable of debonding, and one layer of degraded skin two material. The resulting elements have aspect ratios of 1:1:3 in the hot skin and the debonding layer, 8:1:3 in the core, and 2:1:3 in the cold skin.

Figure 9.1 shows the stable (relaxed) configuration of three models—these represent the panel with 31.8 mm of insulation and loaded with 43.8 N/mm after 10, 15, and 20 minutes of exposure to the fire. Figure 9.2 shows the out-of-plane displacement predictions that result from a series of these models. Clearly of the four panel configurations, only the panel with 31.8 mm of insulation and loaded with 43.8 N/mm will fail during the thirty minute simulation, and this panel will fail just after twenty minutes of exposure. Thus the failure mode observed at twenty minutes in Figure 9.1, global (Euler) buckling, represents the failure mode of the panel. This is to be expected as the panel is long and relatively slender—
Figure 9.1: Typical structural finite element model—displaced configuration (2× magnification) at 10, 15, and 20 minutes. Panel has 5/8” (31.8 mm) of insulation, and is loaded with 3 kip/ft (43.8 N/mm).

Figure 9.2: Predicted out-of-plane deflections with time (failure in Euler macrobucking).

one would expect a failure mode of plastic microbuckling to occur in more short, stubby panels.
Table 9.1: Temperature and displacements readings

<table>
<thead>
<tr>
<th></th>
<th>0 min.</th>
<th>30 min.</th>
<th>60 min.</th>
<th>65 min.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposed face temp. (°C)</td>
<td>15.2</td>
<td>53.5</td>
<td>97.7</td>
<td>112.6</td>
</tr>
<tr>
<td>Mid-point temp. (°C)</td>
<td>15.2</td>
<td>44.7</td>
<td>85.4</td>
<td>90.2</td>
</tr>
<tr>
<td>Unexposed face temp. (°C)</td>
<td>15.2</td>
<td>37.8</td>
<td>69.6</td>
<td>73.5</td>
</tr>
<tr>
<td>Out-of-plane deflection (mm)</td>
<td>0</td>
<td>2</td>
<td>13</td>
<td>20</td>
</tr>
</tbody>
</table>

9.7 Validation

In this section a separate example is run to validate the structural model. This example uses measured temperatures together with the mechanical property degradation curves defined in Chapter 8 to verify the behavior of the finite element structural models. The experimental result was obtained previously [5]. In particular, a single-skin fiber reinforced polymer (FRP) panel was tested, composed of a 56 oz, 5608-08 Quadraxial E-glass fabric, vacuum infused via SCORMPTM with a VEX vinylester matrix, with a fiber density of about 55% by volume. The panel was insulated with two 1.26 kN/m³ (8 lbs/ft³) mineral wool panels, each nominally 25.4 mm thick, on the fire side. Temperatures were recorded via internal thermocouples (placed between the laminae before the fabric was infused with resin) just below the exposed (fire side) face, at the panel midpoint, and just below the unexposed face. These thermocouples resulted in significant warping of the laminae, and likely formed a significant defect in the panel. The panel was pinned at the top and bottom, and free at the sides. The insulated panels were loaded, both in compression and with an out-of-plane load. The out-of-plane load was applied at the unexposed face over an 0.0929 m² area. The loaded panels were then exposed to the ASTM E-119 standard fire temperature curve. Loading was stopped before failure was observed.

The panel was 12.2 mm thick, 914.4 mm long and 711.2 mm wide. It was subjected to a constant 6.67 kN in-plane compressive load, as well as a constant 1.33 kN out-of-plane load at the panel midpoint (pushing in at the cold face). The recorded temperature readings and accompanying out-of-plane displacements are given in Table 9.1. Note that these displacements do not include the initial
The compressive stress component in the lengthwise ($z$) direction for the panel...
(mirrored to appear as a full panel) is displayed in Figure 9.3. Figure 9.4 shows the plastic shear behavior of this panel. Clearly the failure mode is global buckling, as opposed to plastic microbuckling.

Figure 9.3: Typical finite element model—compressive stress component in longitudinal direction (MPa). Note that this panel has an in-plane distributed load as well as an out-of-plane distributed load centered at the panel midpoint.

Figure 9.4: Finite element model, 65 minutes—plastic shear strain. Values below scale provided are uncolored. Note that this panel has an in-plane distributed load as well as an out-of-plane distributed load centered at the panel midpoint.
The structural model displacements were adjusted to incorporate the deflection resulting from the thermal strains. Again, in the model it is assumed that the temperature distribution is linear. The maximum (i.e. midpoint) deflection in a simply supported beam (approximate for the 1/4 panel case, applicable for the plane strain case), with uniform elastic constants, due to an internal linear temperature gradient is given by

\[
\delta_{\text{max}} = \frac{\alpha L^2}{8t} (T_f - T_b)
\]

(9.2)

Note that the only material property that enters is the coefficient of thermal expansion which was assumed to be uniform as an approximation. Here \(\alpha\) is the coefficient of thermal expansion of the panel material, \(L\) is the panel length, \(t\) is the panel thickness, and \(T_f\) and \(T_b\) are the front and back face temperatures, respectively. In fact, this formula is approximately valid even with an accompanying gradient in the elastic modulus through the panel in the absence of mechanical loading. For our purposes \(\alpha\) is taken to be \(1.8 \times 10^{-5} \text{ K}^{-1}\), and the temperature values again are those values taken from the linear regression at the given locations. The resulting thermal deflections are then added to the structural model deflections due to mechanical loading to yield a predicted displacement.

The quarter panel models were quite expensive to solve in terms of computational effort, and so a simplified method of solution was sought. A plane strain model of the same problem was therefore constructed. This model was only one element wide, with plane strain boundary conditions applied. The load was applied within a 0.305 m length at the panel center. All other dimensions, boundary conditions, and material properties were identical to the previous model. The displacements obtained via the full panel model were found to consistently be the displacements obtained via the plane strain model multiplied by a factor of about 1.033. The experimental, full panel model, and plane strain model incremental out-of-plane displacements are given in Table 9.2. The displacements are given as increments above the loaded panel initial \((t = 0 \text{ min.})\) displacements at room temperature.
Table 9.2: Experimental and predicted incremental displacements

<table>
<thead>
<tr>
<th></th>
<th>0 min.</th>
<th>30 min.</th>
<th>60 min.</th>
<th>65 min.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental displacement (mm) (°C)</td>
<td>0</td>
<td>2</td>
<td>13</td>
<td>20</td>
</tr>
<tr>
<td>Thermal deflection (mm) (°C)</td>
<td>0</td>
<td>2.41</td>
<td>4.35</td>
<td>6.03</td>
</tr>
<tr>
<td>Non-thermal deflection (mm) (°C)</td>
<td>0</td>
<td>0</td>
<td>8.65</td>
<td>13.97</td>
</tr>
<tr>
<td>Adjusted deflection (for plane strain, mm)</td>
<td>0</td>
<td>1.94</td>
<td>12.58</td>
<td>19.36</td>
</tr>
<tr>
<td>Adjusted non-thermal deflection (mm)</td>
<td>0</td>
<td>0</td>
<td>8.24</td>
<td>13.33</td>
</tr>
</tbody>
</table>

Table 9.3: Case 1 plane strain model incremental deflections (mm)

<table>
<thead>
<tr>
<th></th>
<th>0 min.</th>
<th>30 min.</th>
<th>60 min.</th>
<th>65 min.</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Adjusted exper. values for reference)</td>
<td>0</td>
<td>0</td>
<td>8.24</td>
<td>13.33</td>
</tr>
<tr>
<td>Typical properties, $E = 20685$ MPa</td>
<td>0</td>
<td>0.23</td>
<td>2.56</td>
<td>4.50</td>
</tr>
<tr>
<td>Beam theory estimate, $E = 9590$ MPa</td>
<td>0</td>
<td>0</td>
<td>15.10</td>
<td></td>
</tr>
<tr>
<td>False position iteration, $E = 16118$ MPa</td>
<td>0</td>
<td>4.04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>False position iteration, $E = 13946$ MPa</td>
<td>0</td>
<td>5.48</td>
<td></td>
<td></td>
</tr>
<tr>
<td>False position iteration, $E = 12932$ MPa</td>
<td>0</td>
<td>6.52</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Estimate, $E = 12000$ MPa</td>
<td>0</td>
<td>0.66</td>
<td>7.85</td>
<td>14.64</td>
</tr>
<tr>
<td>Percent difference</td>
<td></td>
<td>-4.8%</td>
<td>9.8%</td>
<td></td>
</tr>
</tbody>
</table>

9.8 Mechanical property optimization

The plane strain model was used for the optimization problem for computational efficiency. The goal of the problem is to determine how the input parameters used in the material model might account for the discrepancy between the experimental and numerical displacements. The input parameters explored were the elastic constants. The values $c_{11} = 24820$ MPa, $c_{12} = 8274$ MPa, and $c_{44} = 8274$ MPa were obtained using a Young’s modulus of 20685 MPa and a Poisson’s ratio of 0.25. The value of Young’s modulus which would provide for the closest match between the numerical and experimental solutions was sought. An initial guess was obtained via beam formulas for the plane strain case. The guess thus obtained was a value for Young’s modulus of 9590 MPa, with the Poisson’s ratio held constant at 0.25. Then a false position iteration was carried out to yield subsequent guesses as given in Table 9.3. As it was clear the false position iteration was overestimating
the required modulus, the fourth guess was estimated to be a value still lower than the third. This estimated undegraded elastic modulus of $E = 12000$ MPa yielded a satisfactory fit of the experimental data. For this value, the estimated displacement at 60 minutes under by less than 5%, and the estimated displacement at 65 minutes was over by under 10%. This is a significant improvement over the initial model values. This result is shown in Figure 9.5.

![Figure 9.5](image-url)

Figure 9.5: Out-of-plane displacement with time.

Clearly the estimated elastic modulus could account for the discrepancy between the model deflections and the experimental deflections. Yet the elastic modulus that causes the model to match the experimental result should also be shown to be reasonable, or in agreement with values in the literature. Per Mouritz et al. [65], a typical woven glass/vinyl ester composite has a flexural modulus of 17700 MPa. Likewise, a typical woven glass/polyester composite has a modulus of 17800 MPa, and a chopped glass/polyester composite has a modulus of 10500 MPa. We would expect a quadraxial composite to be toward the high end of this range, but clearly a value of 12000 MPa not entirely unreasonable. As was mentioned earlier, the presence of thermocouples served as defects and likely weakened the panel significantly. Thus a combination of their effect and the overestimation of the elastic modulus would fully account for the discrepancy between the predicted
and measured displacements.
Chapter 10

Example application and methodological validation

10.1 Introduction

In this section, a recent test result for a full-panel structure will be used both to validate the current methodology, and as well as an example problem to demonstrate the process put forth in the current dissertation. First, the experimental setup will be described. Then the modelling process will be carried out, step-by-step, and used at each step to validate the current methodology.

10.2 Experimental description

Tests were designed by Professor Robert J. Asaro at UCSD and conducted by Dr. Brian Lattimer at Hughes Associates, Inc. These involved placing FRP composite panels in a loading frame, and exposing them to standard fire temperature curves. In other words, panels were loaded, and the loading maintained while thermal degradation progressed, with temperature and deflection data measured until failure. For the purposes of the current chapter, two of these tests are of interest, in particular two tests performed on single panels. The panels were 20 ply, of quasi-isotropic (quadraxial) lay-up with an overall thickness of 12 mm. The
laminate was fabricated using 24 oz./yd² Vetrotex Certainteed 324-3B 5:4 plain weave E-glass fiber reinforcement with vinyl ester Derakane 510A resin matrix. The panels were 0.917 m (36 in.) high and 0.711 m (28 in.) wide.

The panels were insulated with 25.4 mm (1.0 in.) thick Superwool 607 amorphous glass fiber blanket, 96 kg/m³ (6 lb/ft³) density. They were exposed to the IMO A.754(18) (FTP) fire temperature exposure. Temperatures were recorded in the furnace, at the exterior insulation surface, at the insulation/panel boundary, at 1/3 and 2/3 of the panel thickness (via drilled thermocouples inserted through the cold face), and at the panel cold face. The heat flux was also measured at the exposed insulation surface.

The two tested panels were exposed to the same temperature curve, yet were loaded with different loads. The first panel, single panel #2, was loaded at 9.9 kN. The second panel, single panel #3, was loaded at 4.78 kN for almost 100 minutes. The load was then gradually increased until structural failure was observed. The loading apparatus imposed fix/pin boundary conditions upon the panel. One inch of the panel length was lost in order to achieve the fixed end boundary condition. The in-plane deflection was measured—as well, the out-of-plane deflection was measured at 1/6, 1/3, and 2/3 of the panel length from the pin connection.

## 10.3 Thermal model

In figure 10.1, the thermal model prediction, using the material parameters defined in Chapter 4, is compared with the average measured temperatures. Clearly there are two major discrepancies between the predicted temperatures and the measure temperatures. The first is that the hot face temperatures of the composite panel initially rise much faster than predicted. However, it is apparent that while the furnace temperature tracks the IMO/FTP temperature curve closely, the insulation hot face temperature actually significantly exceeds the furnace temperature, even by as much as 150°C, early in the simulation. No doubt this is a result of significant radiation heat tranfer. This accounts fully for this observed discrepancy.
The second discrepancy is at the cold face. The hot face temperature is hotter than predicted, especially early in the simulation. Thus one would expect this to transfer through and lead to cold face temperatures that are hotter than predicted. However, the cold face does not increase in temperature as quickly as predicted. In fact, the cold face temperature at the end of the simulation ends up being about 50°C cooler than predicted. This should not be due to the thermal model parameters related to decomposition, as the panel temperatures haven’t yet reached the threshold at which decomposition begins at the times in which this behavior is occurring. The properties of the char also shouldn’t account for the discrepancy, as not much char formation has occurred via decomposition. Likewise, the hot face boundary condition parameters are unlikely to account for the discrepancy, as the temperatures at the hot face exceed the predicted values. Thus the parameters which could account for this include $c_{pvb}$, $c_{pvm}$, $\epsilon_c$, $k_{sc}$, $k_{vb}$, $k_{vm}$, and $\rho_v$. Of these, $c_{pvb}$ and $c_{pvm}$ were found in the sensitivity analyses discussed in Chapter 5 to be less
important in determining the temperature prediction, and thus are less likely to account for the discrepancy. The discrepancy could therefore be explained (again with reference to the sensitivity analyses results) by $\epsilon_c$ or $k_{sc}$ being too small, by $k_{vb}$ being too big, by $k_{vm}$ being too small, or by $\rho_v$ being too small.

### 10.4 Thermal deflections

Figure 10.2 shows predicted thermal deflections and as well total measured deflections for the panel with the lightest loading. Note that the predicted thermal deflections are based on the predicted temperatures, which are somewhat different than the actual measured temperatures. Note also that the predicted thermal deflections assume pin/pin boundary conditions. The measured thermal deflection is for a panel with fix/pin boundary conditions—thus one would expect the measured thermal deflection to be scaled down. However, the measured thermal deflection results from a panel subjected to a 4.78 kN in-plane load. One would expect this to magnify the observed out-of-plane deflection. Thus these two discrepancies will likely counteract each other to some degree.

In fact, the agreement between the two, even accounting for the various discrepancies between the predicted and measured data, is very good. Looking at the measured thermal data, one can see that the thermal gradient is not decreasing.
in severity—thus one would not expect the panel to “snap-back” using traditional models for the thermal deflection (as in Equation (9.2)). It is only when one accounts for the degradation of the coefficient of thermal expansion as given in Equation (6.6) that one can reproduce this behavior.

### 10.5 Structural model

The structural model prediction was found to be significantly different from the observed behavior. In particular, the buckling load was significantly under-predicted. Figure 10.3 shows the predicted out-of-plane deflection with time using the full structural finite element models, and as well the Euler buckling load with time using a simplified model.

![Figure 10.3: Predicted out-of-plane deflections, panel loaded with 10 kN in-plane load (left); predicted buckling load degraded per transformed area method (right).](image)

The Euler buckling load with time calculation uses the transformed area method to degrade the panel. In particular, the panel thickness is discretized into a finite number of layers (fifty for the given figure). The width of each layer is then reduced proportional to the ratio of the degraded elastic modulus to the undegraded elastic modulus. The moment of inertia of the resulting cross section is then calculated, and this moment of inertia is used in the Euler buckling equation.

Clearly both results (which use the same predicted thermal data) are in agreement—
per the full structural finite element models, failure occurs via Euler buckling just after twenty minutes for a panel loaded with 10 kN. The simplified model calculation also shows that the Euler buckling load reaches 10 kN after about twenty minutes. Thus the full structural finite element result is verified.

However, in the experiment, the panel failed after just over 62 minutes—so clearly the accuracy of the 20 minute time-to-failure prediction was woefully inadequate. This significant discrepancy is attributed to the fact that the mechanical properties are assumed in Chapter 8 to degrade to a near-zero minimum fraction at temperatures beyond the glass transition temperature. What the observed failure time indicates is that this conservative assumption is to a degree unrealistic. The experimental samples by which this degradation curve were determined were only a few layers in thickness. In the present example, the panel is over twenty fiber layers in thickness. Therefore, there is more to hold the fibers in place, even after the resin has become pliable.

The actual buckling time of 62.73 minutes indicates that at that time—even after the entire panel had passed through the glass transition temperature—the FRP composite still had effectively 24% of its undegraded elastic modulus. Thus while the degradation curves provided in Chapter 8 are conservative, and therefore adequate for design purposes, they significantly underpredict the post–glass transition mechanical properties. Work is currently being completed to address this issue—in particular, this new data is being used to determine more accurate degradation curves. One such curve is depicted in Figure 10.4. This figure utilizes an error function–based degradation curve, as initially proposed by A. G. Gibson et al. at the University of Newcastle. In contrast to their proposal, however; this curve, upon reaching the temperature at which pyrolysis initiates at common heating rates, degrades linearly to a near-zero minimum fraction. Similar curves can be derived using the hyperbolic tangent function and other functions. Work is currently being completed to optimize the fit of such a function to the available experimental data.
Figure 10.4: Degradation curve proposed to alleviate under-prediction of post-glass transition mechanical properties.

10.6 Conclusion

In conclusion, this process has been used to predict the results of an experiment that has subsequently been conducted. The thermal model result was quite accurate, and the observed discrepancies could be accounted for. The thermal deflection model was shown to describe observed phenomena that could not otherwise be accounted for. The description of mechanical property degradation with temperature that was used was shown to be overconservative, leading to the failure predictions of the structural models to be overconservative. However, the structural model result was verified, and new degradation curves are under development to address this inadequacy.
Bibliography


