MODELLING LASER LIGHT PROPAGATION IN THERMOPLASTICS
USING MONTE CARLO SIMULATIONS

By

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Abstract

Laser welding has great potential as a fast, non-contact joining method for thermoplastic parts. In the laser transmission welding of thermoplastics, light passes through a semi-transparent part to reach the weld interface. There, it is absorbed as heat, which causes melting and subsequent welding. The distribution and quantity of light reaching the interface are important for predicting the quality of a weld, but are experimentally difficult to estimate. A model for simulating the path of this laser light through these light-scattering plastic parts has been developed. The technique uses a Monte-Carlo approach to generate photon paths through the material, accounting for absorption, scattering and reflection between boundaries in the transparent polymer. It was assumed that any light escaping the bottom surface contributed to welding. The photon paths are then scaled according to the input beam profile in order to simulate non-Gaussian beam profiles.

A method for determining the 3 independent optical parameters to accurately predict transmission and beam power distribution at the interface was established using experimental data for polycarbonate at 4 different glass fibre concentrations and polyamide-6 reinforced with 20% long glass fibres. Exit beam profiles and transmissions predicted by the simulation were found to be in generally good agreement ($R^2>0.90$) with experimental measurements. The simulations allowed the prediction of transmission and power distributions at other thicknesses as well as information on reflection, energy absorption and power distributions at other thicknesses for these materials.
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# Table of Contents

Abstract............................................................................................................................................. ii  

Acknowledgements.................................................................................................................................. iii  

List of Tables ........................................................................................................................................... vii  

List of Figures ........................................................................................................................................ viii  

List of Symbols ....................................................................................................................................... xi  

Chapter 1.  Introduction.............................................................................................................................. 1  
1.1 Plastics .............................................................................................................................................. 1  
1.2 Laser Transmission Welding .............................................................................................................. 4  
1.3 Thesis Objectives and Outline .......................................................................................................... 6  

Chapter 2.  Modeling Light Propagation through Plastics.......................................................................... 7  
2.1 Overview of Laser Transmission Welding in Polymers ...................................................................... 7  
2.1.1 Transmission .................................................................................................................................. 8  
2.1.2 Scattering ...................................................................................................................................... 10  
2.2 Monte Carlo ....................................................................................................................................... 13  
2.3 Problem Identification and Methodology .......................................................................................... 15  

Chapter 3.  Development of Simulation Model.......................................................................................... 16  
3.1 Monte Carlo Method for Photon Transport ...................................................................................... 16  
3.1.1 Program Initialization ..................................................................................................................... 18  
3.1.2 Photon Positioning and Initial Conditions .................................................................................. 19  
3.1.3 Photon Step .................................................................................................................................. 20
5.1 Equipment and Materials ................................................................. 55
5.2 Minima Search Algorithms .............................................................. 57

Chapter 6. Using the Simulation to Reproduce Experimental Data .................. 59

6.1 Polycarbonate .................................................................................. 59
6.1.1 PC10GF ..................................................................................... 59
6.1.2 PC15GF ..................................................................................... 64
6.1.3 PC30GF ..................................................................................... 68
6.1.4 PC40GF ..................................................................................... 70
6.1.5 Polycarbonate Results Summary .................................................. 72

6.2 Polyamide-6 ................................................................................... 77
6.2.1 Polyamide-6 Results Summary ..................................................... 82

Chapter 7. Conclusion ......................................................................... 85

7.1 Recommendations ........................................................................... 85

Bibliography ......................................................................................... 87

Appendix A ............................................................................................ 93
Appendix B ............................................................................................. 101
Appendix C ............................................................................................. 106
Appendix D ............................................................................................. 109
Appendix E ............................................................................................. 111
PA-6 ....................................................................................................... 111
PC40GF ................................................................................................. 112
List of Tables

Table 4-1 Photon in/out counts for $10^2$-$10^5$ photons .......................................................... 34
Table 4-2 Simulation parameters used in each trial ........................................................................... 44
Table 5-1 Osterman polycarbonate (PC95X series) samples used ....................................................... 56
Table 6-1 Simulation solutions for PC10GF ...................................................................................... 63
Table 6-2 Simulation solutions for PC15G ...................................................................................... 67
Table 6-3 Transmission values for PC30GF at two thicknesses ......................................................... 70
Table 6-4 Simulation solutions for PC30GF ...................................................................................... 70
Table 6-5 Transmission data for two thicknesses of PC40GF ............................................................. 72
Table 6-6 Optical Parameters determined for PC40GF ................................................................. 72
Table 6-7 Simulation solutions for PA6-LGF20% ........................................................................... 82
Table 0-1 Portion of brute force data for PA-6 ............................................................................... 111
Table 0-2 Portion of brute force data for PC30GF .......................................................................... 112
List of Figures

Figure 1-1 Modulus vs temperature for PC and PBT [3]........................................................................................................... 2
Figure 1-2: Generic laser transmission lap weld......................................................................................................................... 4
Figure 2-1 Laser scattering through PA-6, PA-46 and PBT [22] .................................................................................................... 10
Figure 2-2 Thermal imaging of a PA-6 Lap-Joint [24] .................................................................................................................. 11
Figure 3-1 Flowchart summary of the Monte Carlo Method for Photon Transport ................................................................. 17
Figure 3-2 Simulation block concept diagram.......................................................................................................................... 19
Figure 3-3 Coordinate system showing azimuthal and deflection angle definitions .............................................................. 22
Figure 3-4 Two-dimensional beam profile for the Rofin laser system, in focus ............................................................... 28
Figure 3-5 Two-dimensional beam profile for the Rofin laser system, 3mm below focus....................................................... 29
Figure 3-6 Original beam profile data, left, and S, the interpolated data matching the resolution used in the
Monte Carlo simulation ....................................................................................................................................................... 30
Figure 3-7 Filling the MZ master matrix by scaling point source data, according to the values of the beam
profile “S” ........................................................................................................................................................................ 32
Figure 4-1 Simulation of Beer's law behaviour for varying absorption coefficients ....................................................... 36
Figure 4-2 Concept of obtaining the T-PFD .......................................................................................................................... 38
Figure 4-3 Effect of scattering coefficient and photon count on simulation runtime ................................................... 39
Figure 4-4 Effect of photon count on sequential value of $A_{rss}$ ............................................................................................. 40
Figure 4-5 T-NPFD for a point source beam, multiple values of $N_{photons}$ ..................................................................... 41
Figure 4-6 Effect of resolution (number of bins) on program runtime .................................................................. 43
Figure 4-7 T-NPFD for a point source of light as a function of $g$ ....................................................................................... 45
Figure 4-8 T-NPFD for an in-focus Rofin laser as a function of $g$ .................................................................................. 46
Figure 4-9 Transmission as a function of $g$ ......................................................................................................................... 47
Figure 4-10 T-NPFD for a point source as a function of $\mu_s$ .............................................................................................. 48
Figure 4-11 T-NPFD for an in-focus Rofin laser as a function of $\mu_s$ ............................................................................... 48
Figure 4-12 Transmission as a function of $\mu_s$ ................................................................. 49
Figure 4-13 T-NPFD for a point source as a function of $\mu_a$.................................................... 50
Figure 4-14 T-NPFD for an in-focus Rofin laser as a function of $\mu_a$........................................ 51
Figure 4-15 Transmission as a function of $\mu_a$ ........................................................................ 52
Figure 4-16 T-NPFD for an in-focus Rofin laser as a function of $n_{mat}$ ....................................... 53
Figure 4-17 Index of Refraction versus Transmission ............................................................... 54
Figure 5-1 Laser scan lines produced on the sensor polymer using a 2.2mm PA6-20%LGF sample as the top part ......................................................................................................................... 56
Figure 6-1 T-NPFD for an in-focus Rofin laser scattered by a 2.3 mm PC10GF plate .................... 60
Figure 6-2 T-NPFD for an in-focus Rofin laser scattered by a 3.2 mm PC10GF plate .................... 61
Figure 6-3 Transmission versus thickness for PC10GF plates, simulated and experimental ........ 62
Figure 6-4 $\ln T_T$ vs. D for PC10GF.......................................................................................... 63
Figure 6-5 T-NPFD for an in-focus Rofin laser scattered by a 2.3 mm PC15GF plate .................... 64
Figure 6-6 T-NPFD for an in-focus Rofin laser scattered by a 3.2 mm PC15GF plate .................... 65
Figure 6-7 Transmission versus thickness for PC15GF plates, simulated and experimental ........ 66
Figure 6-8 $\ln T_T$ vs. D for PC15GF.......................................................................................... 67
Figure 6-9 T-NPFD for an in-focus Rofin laser scattered by a 2.6 mm PC30GF plate .................... 68
Figure 6-10 T-NPFD for an in-focus Rofin laser scattered by a 3.2 mm PC30GF plate................... 69
Figure 6-11 T-NPFD for an in-focus Rofin laser scattered by a 2.2 mm PC40GF plate .................. 70
Figure 6-12 T-NPFD for an in-focus Rofin laser scattered by a 3.1 mm PC40GF plate .................. 71
Figure 6-13 T-NPFDs for each 3.2mm polycarbonate plate tested............................................. 73
Figure 6-14 Beam profile distributions for PC15GF at various thicknesses, zoomed for clarity ........ 74
Figure 6-15 Variation in optical parameters as glass fibre concentration increases; values in mm$^{-1}$ where applicable .................................................................................................................. 75
Figure 6-16 Laser light absorption within a 3mm (top) and 6mm PC30GF (bottom) part, XZ cross section ........................................................................................................................................ 76
Figure 6-17 T-NPFD for a 1.5mm PA6 20%GF sample, experimental and simulated ........................................77
Figure 6-18 T-NPFD for a 2.2mm PA6 20%GF sample, experimental and simulated .................................78
Figure 6-19 T-NPFD for a 3.1mm PA6 20%GF sample, experimental and simulated ...............................79
Figure 6-20 Transmission for varying PA6-LGF20% thicknesses, simulated and experimental ...............80
Figure 6-21 lnT_T vs. D for PA-6-LGF20% ..................................................................................................81
Figure 6-22 T-NPFD for PA6-20%LGF at various thicknesses ...................................................................83
Figure 6-23 Laser light absorption within a 3mm and 6mm in PA-6 20%GF, XZ cross section ..............84
List of Symbols

\( T_g \)  Polymer glass-transition temperature

\( T_m \)  Polymer melting temperature

\( \mu_a \)  Absorption coefficient, 1/mm

\( \mu_s \)  Scattering coefficient, 1/mm

\( \mu_k \)  Extinction coefficient, 1/mm

\( I \)  Light intensity, W/m\(^2\)

\( A_I \)  Apparent absorption coefficient, 1/mm

\( R_T \)  Total reflection

\( T_T \)  Total transmittance

\( \eta \)  Surface reflectance

\( D \)  Depth, mm

\( \Psi \)  Transverse normalized power flux distribution, 1/mm

\( \Psi^* \)  Scaling factor

\( w_k \)  Weld line thickness, mm

\( \delta \)  Scattered light fraction

\( \sigma \)  Scattering standard deviation

\( N_x \)  Number of bins, x axis

\( N_y \)  Number of bins, y axis

\( N_z \)  Number of bins, z axis

\( X_0 \)  Block length along x axis, mm

\( Y_0 \)  Block length along y axis, mm

\( Z_0 \)  Block length along z axis, mm

\( \Delta x \)  Resolution x direction, mm
Δy Resolution y direction, mm

Δz Resolution z direction, mm

N_{\text{photons}} Number of photons

\( w \) Initial photon weight

\( w_t \) Photon weight threshold

\( \xi \) Uniform random number on [0,1].

\( u_x \) Photon direction cosine, x direction

\( u_y \) Photon direction cosine, y direction

\( u_z \) Photon direction cosine, z direction

\( Q \) Absorption matrix

\( \phi \) Azimuthal angle, degrees

\( \theta \) Deflection angle, degrees

\( g \) Anisotropy factor

\( n \) Index of refraction

\( R_p \) Fresnel reflection coefficient, p-polarized light

\( R_s \) Fresnel reflection coefficient, s-polarized light

\( R \) Fresnel reflected portion

\( T \) Fresnel transmitted portion

\( S \) Interpolated beam profile, 1/mm²

\( A_{rss} \) Objective difference
Chapter 1. Introduction

Examples of commonly used engineering plastics include polypropylenes, polycarbonates and polyamides (commonly known as nylons). The processes for efficiently producing these materials were developed during the 20th century and the relative abundance of raw materials, along with their adaptability, means that they are now used everywhere on earth, in almost every application imaginable. They are extensively used in construction, clothing, electronics and transportation industries. Development of plastic joining technologies, then, must keep up with the expanding capabilities of these dynamic materials.

1.1 Plastics

Plastics can be divided into two categories. Thermoset plastics, like epoxy resin, typically flow with relative ease at room temperature as a ‘sea’ of monomers. These materials must be cured, primarily through heat (hence thermo), though some may be cured through exposure to radiation. In curing, polymer chains form, are cross-linked irreversibly, and the material hardens. Thermosets typically have very good material properties, but their inability to soften or melt at an elevated temperature means that their applicability to heat-welding is limited [1].

This thesis will focus on thermoplastics. Thermoplastics can be successfully subjected to a variety of heat-treatments. These plastics are further subdivided into amorphous or semi-crystalline materials. Amorphous polymers have all of their molecules in an amorphous phase which is thoroughly unordered. These materials are typically clear or quite translucent, as there are no regular structures to appreciably scatter light.

Semi-crystalline thermoplastics, by contrast, have some portions of their polymer chains crystallized, and are typically characterized by their percent-crystallinity. Factors influencing crystallinity include the chemical structure of the polymer, though some materials may never crystallize, due to their molecular
geometry. Treatment during manufacture is also a factor; crystal growth may be controlled by temperature. Materials that may otherwise crystallize may be inhibited from doing so by rapid cooling, known as quenching [2].

Common to both classes of thermoplastic is the glass transition temperature, $T_g$. Below the glass transition temperature, the mechanical properties of the plastic are largely consistent, but above, its characteristics change drastically. Above the $T_g$, amorphous phase molecules are no longer frozen and have enough energy to change their conformation, displaying liquid-like behaviour while remaining entangled. Crystalline phases remain crystallized, preserving some of their solid-state properties. Further heat must be added to melt these crystal structures at the melting temperature, $T_m$, which results in the loss of any remaining strength. Figure 1-1 shows the Modulus versus Temperature relationship for polybutylene terephthalate (semi-crystalline) and polycarbonate (amorphous) thermoplastic.

![Figure 1-1 Modulus vs temperature for PC and PBT][3]
Additionally, reinforcement of these thermoplastics may also be considered. Glass or carbon fibres are often added during manufacturing to increase the overall strength and stiffness of the material. This typically does not greatly affect either the $T_g$ or the $T_m$ [2].

Thermoplastics are most commonly formed by injection molding, where hot plastic is injected into a mould, cooled and removed. In the case of semi-crystalline materials, the cooling times and temperatures are carefully monitored to control the overall level of crystallization, as well as to avoid warping of the parts caused by unequal rates of cooling [4]. Joining parts after injection moulding may be required for various reasons. These can include the manufacture of hollow casings or housings, or complex shapes and overhanging geometries. Techniques for joining plastic parts fall into three broad categories: mechanical fastening, adhesion or welding.

The use of mechanical fasteners to join components is widely adopted and immediately apparent on many consumer plastic products. Either metallic or plastic fasteners, such as clamps, screws or bolts, are used to fasten mating geometries. While mechanical fasteners work well to allow the joint to be reopened or replaced, stronger plastics are required due to the high stresses that typically surround the fastener [5].

Adhesion, the second broad category of joining plastics, involves using a chemical adhesive to glue two mating surfaces together. Adhesives made from thermosetting materials, like epoxy, are common.

Welding, the third technique, uses the material itself for joining, and works by heating the local weld area to produce a phase change in the material at the weld interface, causing local heating, melting and subsequent welding. Several specialized techniques exist for inducing this localized heat. There are direct methods, such as hot plate or hot gas welding, which use heated media to transfer energy to the plastic weld interface, and friction methods, which use high frequency vibrations or friction between components to quickly produce welds. The final class of methods, using electromagnetic radiation, includes infrared welding and laser transmission welding.
1.2 Laser Transmission Welding

Transmission welds are made by bringing the two parts to be joined together along their mating faces. The top part, known as the transmitting part, must transmit a significant fraction of radiation at the wavelength of the laser used. The bottom piece, the absorbing part, is made of either the same or another compatible material, but contains a laser-absorbent such as carbon-black. With the parts in close contact, the laser energy passes through the transparent part to the weld-interface, where the radiant light is absorbed. The heating that results is partly conducted to the transparent part, and melting of both parts results in diffusion of molecules across the interface, which produces the weld. Figure 1-2 below shows a simple schematic of a laser lap weld.

The lasers used are typically in the near-infrared spectrum, as at these wavelengths, many polymers are relatively transparent [6]. Diode lasers are common due to their efficiency and weight, though Nd:YAG and fibre lasers are also used [7].

Several techniques are used industrially to deliver laser energy to the assembly. So-called contour welding involves the laser slowly tracing the weld pattern across the parts to be joined. It is used on large...
parts that are in good contact with one another. The weld interface will see only a single pass of the laser. In *quasi-simultaneous* welding, the laser rapidly scans the welding surface, usually using mirror galvanometers, in an attempt to uniformly heat and melt the mating surfaces and minimize localized stresses or poor contact due to uneven thermal expansion. Finally, *simultaneous* welding uses multiple laser sources to irradiate the joint simultaneously. This may be the least adaptable of the techniques as changes to geometries of the part may require changes to the geometry of the working area and laser configurations.

Although the concept of using lasers to transmission-weld plastic polymers was conceived in 1985, it would take until 1997 for Mercedes to become the first company to use the technique on a mass production-scale, fabricating keyless entry devices for their vehicles [8]. In 1998, the Clearweld process was patented. This process replaced the black, absorbing part with a visibly transparent, light-absorbing resin sandwiched between the parts, with the aim of preserving a visibly clear joint.

Generally, laser welding times are fast compared to other joining methods [7]. Welding of three dimensional geometries is also possible. Other advantages of this method include no contact of heating elements with the weld surface; no part movement or vibration during welding and precise control of the laser power to avoid material degradation. Reliability of the spot-size permits control of the heat-affected zone, and reduction of flash. Prediction of the quantity of transmitted light and its distribution after transmission through the transparent part, however, is complicated.

The transparency of the upper part is of paramount importance in these laser welding techniques. Without a sufficiently transparent material, the power flux reaching the interface may be too low to melt the polymer and produce a weld. Alternatively, to overcome absorption losses, so much power may be required that undesirable heating and decomposition in the transmitting material may occur. In addition to power transmission issues, there can be problems related to laser light scattering. Light reaching the interface is more diffuse, and the distribution of intensity from the original beam has changed. Therefore,
the accurate prediction of the width and strength of a weld is complicated. Scattering is most common in semi-crystalline polymers as well as in composite materials, due to the presence of multiple phases.

While the thermal properties of thermoplastics are fairly well studied and examined, comparatively little work has been done on the investigation of the optical properties of these materials, a key component of the laser-transmission welding process.

1.3 Thesis Objectives and Outline

This thesis aims to develop a model for predicting the scattering of laser light through the transparent part. The model should be capable of determining the exit beam profile distribution, transmission and the absorption of energy as well as total reflection at the incident surface. A successful model would allow its predictions to be used in thermal models of laser welding processes. This will help predict whether areas of transmission weld may undergo thermal degradation due to local heating, as well as predict weld strength and width.

Chapter 2 presents a literature review of previous work on light scattering in polymers, while Chapter 3 describes the model programming code implementation, developed using MATLAB and largely based on the Monte Carlo numerical simulations originally proposed in 1983 by Wilson and Adams [9] for modeling light transmission in biological tissue.

Chapter 4 shows some of the capabilities of the program, including some validation and preliminary results. Chapter 5 addresses the techniques utilized for using the simulation with experimental data, while Chapter 6 presents the results of actual simulations.

The complete listings of program code written are located in the appendices.
Chapter 2. Modeling Light Propagation through Plastics

Section 2.1 of this chapter will review Laser Transmission Welding (LTW) in polymers. It will discuss previous studies on laser transmission including the optical characterization, such as transmittance and reflectance of various materials, including nylon [7] and polycarbonates [10]. Several techniques for measuring scattering at the weld interface include the method established by Zak [11], which uses sequential line scans at increasing thickness and an analytical model proposed by Chen [12] [13] to describe scattering at the interface along a single dimension. Section 2.2 will review Monte Carlo modeling, specifically the work of Ilie [14] [15] [16] who proposed the use of a Monte Carlo technique in LTW as well as the work of Wilson and Adams [9] who examined laser scattering effects in tissue.

2.1 Overview of Laser Transmission Welding in Polymers

Lasers used in LTW typically operate in the near-infrared spectrum, and include diode lasers. Industrial diode lasers consist of tens, or hundreds, of diode laser emitters arranged on heat sinks in “laser bars”. Several of these laser bars make up diode stacks, which are further focused by lenses into a single laser beam. Nd:YAG lasers are also used in laser transmission welding applications. These lasers use a neodymium-doped yttrium aluminium garnet crystal as a lasing medium, and also operate in the near-infrared range, 1064nm [8].

Evaluating the light intensity distribution of an asymmetric laser beam, or beam profiling can be done mechanically, by a pinhole technique. A piece of material with a small hole is placed at the extreme edge of the beam spot, and the laser is shone at a fixed power. Light passing through the aperture is measured with a power meter, and the pinhole is shifted a fixed distance in X or Y and the procedure repeated. Characterization of a Rofin laser was done using a pinhole of 200µm by Mayboudi et al. [17], who described the two-dimensional beam profile at various working distances, including the focal plane.

The optical characteristics of the polymers and their interaction with specific wavelengths can significantly affect the performance of a polymer LTW system. The key optical phenomena are
Transmission, scattering, reflection and absorption. Transmission is the fraction of incoming light making it through the transparent part. Scattering is used to describe the spreading of laser beam as it passes through the transparent part and thus affects the distribution of the transmitted light. Reflection is the fraction of incoming light escaping through the top surface. It is made up of light reflected off the top incident surface, as well as backscattered light. Absorption describes the light that never escapes the transparent part and is instead absorbed and transformed into heat. Total transmission, total absorption and total reflection are typically expressed as percentages of the incident (incoming) light power.

2.1.1 Transmission
For low or non-scattering polymers, the Beer-Lambert-Bouguer Law, or Beer’s Law, is used to estimate the intensity a beam of light as a function of depth according to

\[ I(z)_{\text{Beers}} = I_0 e^{-\mu_k z} \]  

(1)

where \( I(z) \) is the laser intensity (power flux) at a depth \( z \), \( I_0 \) is the intensity at \( z = 0 \), and \( \mu_k \) is the attenuation or extincion coefficient, which is the sum of two coefficients:

\[ \mu_k = \mu_a + \mu_s \]  

(2)

\( \mu_a \) is the absorption coefficient and \( \mu_s \) is the scattering coefficient. In non-scattering polymers, \( \mu_s = 0 \) and \( \mu_k = \mu_a \) [18].

In 2009, Chen [13] presented a modification to the Beer-Lambert-Bouguer Law to improve its utility in the estimation of transmission in scattering polymers. It was proposed that the ratio of power out to power in, or transmission, could be calculated as

\[ \frac{P_{\text{out}}}{P_{\text{in}}} = (1 - R_T)(1 - \eta)e^{-\mu_k D} \]  

(3)

where \( D \) is the sample thickness, \( R_T \) is the total reflection from both the material volume and the top surface and \( \eta \) is the polymer surface reflectance given at the bottom of the laser exiting surface (or weld
interface). $A_1$ is the apparent laser absorption coefficient, an overall measure of a polymers capability of absorbing light. To simplify the calculation, Chen’s assumption was that, despite scattering, light always travelled its initial direction.

Measuring transmission has been done in multiple ways. By using a spectrophotometer, combined with an integrating sphere, Aden et al. [10] examined the effect on transmission of additives such as talc and glass fibers in polycarbonate as a function of wavelength. By using a four-flux model with a spectroscope, Aden estimated a scattering coefficient for 15% glass fiber filled polycarbonate of around 0.8 mm$^{-1}$ in the near-infrared range, decreasing with glass fibre content. Wang et al. [19] also utilized a spectrophotometer with an integrating sphere to estimate transmittance in polyamide, polycarbonate and polypropylene samples at multiple thicknesses and showed that transmittance in thicker samples was lower, due to increased scattering. Kagan et al. [7] utilized near-infrared spectroscopy (NIR) to measure transmission in polyamides. With short glass fibre reinforcements, it was determined that transmission decreased monotonically, due to increased light scattering. Distance to the detector may have resulted in the transmission values measured being lower than expected.

Another method for measuring transmission is the use of a portable power meter. Dosser et al. [20] used a laser power meter placed at 0.5 inches from a sample to examine transmission in carbon nanocomposite particles in matrices of polyetheretherketone (PEEK) and polycarbonate at multiple thicknesses. Results showed that PEEK had a higher attenuation coefficient at 810 and 1064nm. Azhikannickal et al. [21] used the technique to determine transmission in polyamide-6 and glass-filled polycarbonate as a function of angle of incidence and sample thickness. It was found that transmission decreases as the laser incident angle increases. Distance to the power meter was varied, and it was determined that a sample-power meter separation of less than 2mm was necessary to fully capture the total transmitted power.
2.1.2 Scattering

Light passing through polymers is scattered, via reflection and refraction, off any of the spherulites, fibres, pigments and various other chemical additives in a particular polymer formulation. Scattering was shown to increase strongly with the thickness of semi-crystalline polymers and glass fibre content. As a result, the prediction of the beam profile is difficult. Vegte et al. [22] imaged scattering through semicrystalline polyamide and polybutylene terephthalate (Figure 2-1).

![Figure 2-1 Laser scattering through PA-6, PA-46 and PBT [22]](image)

The figure shows the relative scattering of a beam scattered by polyamide-6, polyamide-46 and polybutyleneteraphthalate samples of the same thickness, taken by an infrared camera placed directly underneath each sample. It can be seen that, compared to PA-6, PBT is a highly scattering material, with a much broader transmitted beam distribution.

Mayboudi et al. [23] [24] used thermal imaging techniques to verify a thermal model of the heat distribution at the weld interface (Figure 2-2).
The thermal image shows a heat distribution in the section of a lap weld. Conduction of heat within the weld makes it difficult to estimate scattering, so these images are an indirect observation of light scattering.

Due to the difficulty of beam profiling, several techniques have been developed to estimate the power distribution at the weld interface. A novel technique presented by Zak et al. [11] estimates the Transverse Energy Density Distribution (TEDD) of the laser light at the weld interface. The technique uses a laser-absorbent part to record the width of melted polymer scan lines at progressively higher powers, after the laser light has passed through the transparent part being tested. Starting with the lowest possible power that produces a visible scan line of molten polymer, \( P_0 \), new scans are made as the power is increased incrementally. The result is a progressively wider scan line, as the tail ends of the scattered beam contain the power necessary to melt the absorbent part. Each power used, \( P_k \), is associated with a weld line of a certain width, \( w_k \). The distribution has the normalization requirement that its integral is unity, given by:

\[
\int_{-\infty}^{\infty} \Psi(x) \, dx = 1
\]  

(4)
The transverse normalized power flux distribution (T-NPFD), \( \psi(y) \), is ultimately described by

\[
\psi\left(\frac{w_k}{2}\right) = \frac{P_y \psi'(0)}{P_k}
\]

(5)

\( \psi'(0) \) is the scaling factor required to make the area under the distribution equal to unity.

One shortcoming of this technique is that as the power is increased to obtain wider weld lines, a limit is imposed either by the maximum power available from the laser or by the thermal degradation of the transparent material. Therefore, it is difficult to estimate the tail ends of the distribution. An analytical model developed by Chen et al [12] addresses this limitation. The model discretizes the incoming beam along one direction into many “small point beams”, each having a T-NPFD at the incident surface of denoted \( \Psi_i(x_i, 0) \). He suggests that some portion of the light, \( \delta \), is scattered component, while the fraction \( 1-\delta \) is unscattered, or direct. This direct component is light assumed to pass directly through the material, without scattering, and is proportional to the discretized beam directly above it. Thus, the direct component of the beam at a depth \( D \) is:

\[
\Psi_i(x_i, D)_{\text{direct}} = (1 - \delta) \ast \Psi_i(x_i, 0)
\]

(6)

The scattered component is made up of the overlapping of Gaussian functions centered at each of the small point beams with a common scattering standard deviation of \( \sigma \).

\[
\Psi_i(x_i, D)_{\text{scattered}} = \frac{\delta \ast w_i}{\sqrt{2\pi} \sigma} \sum_{j=-\infty}^{j=\infty} \Psi_i(x_j, 0) e^{-\frac{(w_k - x_j)^2}{2\sigma^2}}
\]

(7)

The transmitted beam, therefore, is proposed to be the sum of these two parts,

\[
\Psi(x, D) = \Psi(x, D)_{\text{direct}} + \Psi(x, D)_{\text{scattered}}
\]

(8)

Using two material dependent parameters, \((\delta, \sigma)\) the above model can be fitted to the line scan data missing distribution tails, the area under the curve can be calculated. The distribution can be normalised, and the missing tail ends can be approximated.
To measure scattering at the weld interface, Becker and Potente [25] used a pinhole profiling technique similar to the approach used by Mayboudi [17] to describe the transmitted laser intensity distribution. A pinhole with an aperture of 1mm was used to measure a beam with an unscattered diameter of 4mm, indicating the resolution limitations of this approach. Additional problems with the total measured power might be caused by light escaping the transparent part at shallow angles, and thus remaining unrecorded by the pinhole.

Haberstroh et al. [26] demonstrated the viability of infrared thermography in beam profiling. An infrared camera was used to image the beam upon entry and exit of the transparent part, made from various polyamides, at different concentrations of glass fibres. The images demonstrated increased scattering as crystallinity and glass fibre concentration increase. Heating of the transparent part observed by Haferkamp et al. [27] indicates the disadvantage of this ‘CCD’ method as conduction over time will increase the apparent beam area, leading to a false image of the beam profile distribution.

2.2 Monte Carlo

Broadly speaking, the so-called Monte-Carlo simulations refer to computer simulations that make use of random numbers. Typically, random numbers are used to change experiment parameters, varying the outcome until a statistical pattern begins to emerge. Real world applications of the Monte Carlo techniques include ray tracing in computer graphics, where light rays are traced along random paths. Other uses include artificial intelligence for video games, and in finance for examining possible outcomes of investments.

The use of stochastic simulations to model light propagation dates back to the 1960s, when Collins and Wells [28] developed computer programs for the US Army electronics command for studying aerosols in the atmosphere. Their codes, written in FORTRAN, were verified using established calculations for determining the atmospheric phenomena simulated. Using the Collins-Wells model, Kattawar and Plass studied the polarization of scattering light in 1968. [29]
In 1983, Wilson and Adam [9] proposed the first modern Monte Carlo technique for measuring the transport of light in tissue for use in the planning of photo radiation therapy, a type of cancer treatment that uses locally-placed, light-activated chemicals to combat malignant tissue [30]. Their model imagined a flat beam, where each photon initially pointed directly into the tissue, or an optical fibre delivery, where each photon would begin with a random, forward angle. Each photon steps over a path length, determined pseudo-randomly, and a fraction of its “weight” absorbed along every step. The scattering direction is updated after each step randomly. The reflection off interfaces was not accounted for. Instead they assumed any backwards directed rays leaving the material were lost. Simulation parameters, such as the mean free path, were estimated based on observations of the behaviour of light in mammalian tissue.

Prahl et al [31] adopted the proposed Monte Carlo technique to model light scattering in multiple layers of tissue. Photon scattering in Prahl’s model is determined by the Henyey-Greenstein (HG) function [32], introducing anisotropy. Also introduced was the use of the Fresnel equations to properly redirect and split light interacting at boundaries. The Prahl model adopted a Cartesian coordinate system, but recorded internal absorption and distribution as functions of r and z, in a cylindrical system with a shared z-axis. In 1995, Wang et al [33] suggested the use of this advanced model to simulate light scattering in multiple tissue layers with unique properties. A summary of the optics of tissue, including a summary of the Monte Carlo method for photon transport is given Chapter 5 of the text Optical-Thermal Response of Laser-Irradiated Tissue, by Welch et al. [34].

In 2005, Ilie et al. [14] were the first group to adopt the technique for simulating light transport in polymers. Their 2007 paper [15] provided further description of their simulation. The authors utilized a simulation in which absorption is ignored, focusing instead on the scattering of the beam as it traverses the part. The direction of photon scattering, rather than using the HG function, was simulated using Mie theory, to simulate light scattering off particles within the plastic matrix. Questions can be raised about the viability of the use of the Mie solutions in this type of simulation. For example, they note that two media containing particles of diameter 0.5μm and 1.24μm results in a photon scattering direction between
0 and 50 degrees, and 0 and 20 degrees respectively. Polymers containing multiple additives – and thus particles of multiple sizes – might be very challenging. They write

*Perceiving the complexity of the issue it is desirable to integrate these factors into a more global parameter in order to facilitate the characterization of the optical properties of a medium*

Additionally, only a Gaussian beam is simulated, with photons launched from a position defined by an angle $\phi$ distributed on $[0,2\pi]$ and a radius $r$ according to the normal distribution.

### 2.3 Problem Identification and Methodology

The estimation of laser scattering and transmission in semitransparent polymers is a problem of great interest in laser welding. Not all input beam profiles are Gaussian, not all polymers are identical and not all parts are the same shape. Therefore, this project aims to develop a computer model that can use a two-dimensional input beam profile to accurately predict (1) the two-dimensional beam profile distribution at the weld interface, (2) total transmission and reflection, (3) internal heat distribution using a Cartesian coordinate system.

MATLAB is used for this task. Though other languages can, in some circumstances provide better processing times [35], MATLAB was chosen primarily for its ease of use when working with matrices, as well as the wealth of functions provided by its various toolboxes and libraries.
Chapter 3. Development of Simulation Model

The laser propagation simulation presented in this thesis consists of three parts. The first part uses the Monte-Carlo method outlined to produce a statistical distribution of light from a single point source passing through the weld interface, as well as at any of the other volume boundaries. This method also provides a statistical distribution of absorbed photons within the part itself and is described in Section 3.1. The second part of the program works by using the Monte-Carlo results to emulate a specific beam profile as different lasers have different power distributions. As discussed in Section 2.1, not all beams are necessarily Gaussian shaped, so the equivalent output beam shape must be simulated by correcting for the input beam. This is discussed in Section 3.2. The third piece of the simulation, discussed in Chapters Chapter 5 and Chapter 6, involves the comparison of simulation results to experimental data. By tuning the optical parameters to match experimental data, the simulation can be used to predict the output beam distribution for materials of varying thickness, as well as varied geometries – where the laser is particularly close to a part edge, for example.

3.1 Monte Carlo Method for Photon Transport

The Monte Carlo simulation described in this thesis tracks paths of light through a medium, and is adapted from the outline provided by Welch et al. [34], based on the method outlined by Wilson et al. [9]. The essence of the technique is presented as a flowchart in Figure 3-1. A photon is initialized, and moved progressively, in steps, through a volume. The photon deposits a fraction of its energy at each step. Each step direction and length is chosen randomly, with the probability of a given direction or length determined by the simulation input parameters. Reflections at material-air boundaries are considered, and as photons’ interactions increase, so does the probability of their removal from the simulation.
Figure 3-1 Flowchart summary of the Monte Carlo Method for Photon Transport
3.1.1 Program Initialization

Here, the geometry of the simulation is established. The program simulates a block of light-scattering plastic in space, so here its dimensions are defined as $X_0$, $Y_0$ and $Z_0$, in millimeters, and the respective resolutions $\Delta x$, $\Delta y$ and $\Delta z$ are chosen such that

\[
N_x = \frac{X_0}{\Delta x}
\]

\[
N_y = \frac{Y_0}{\Delta y}
\]

\[
N_z = \frac{Z_0}{\Delta z}
\]

where $N_x$, $N_y$ and $N_z$ are integers representing the number of bins along each of the Cartesian direction. These numbers can vary from the tens, for low resolution cases, into the hundreds or thousands, depending on the accuracy required. These bins are used to record partial absorption by the material as photons are scattered. Figure 3-2 represents a simple system where $N_x = N_y = 10$, and $N_z = 3$. A matrix, labeled Q, with dimensions $N_x$, $N_y$ and $N_z$ is used to represent the block. Also established are the six “face” matrices, $F_X$, $F_X0$, $F_Y$, $F_Y0$, $F_Z$ and $F_Z0$. These matrices record photons escaping the material across the noted plane – for instance, $F_X0$ records photons that leave the material through the $YZ$ plane where $x = 0$. $F_X$, by comparison, records escapes at the other limit, where $x = X_0$.

It should be noted that, while many Monte Carlo simulations of this nature make use of a radial coordinate system, a Cartesian system is used here. Radial systems cite reduced demands on computer memory, as only information for $Z$ and $R$ needs to be recorded. However, this approach limits the model to a system that is symmetric about $Z$, and is useful only on a machine that is fairly limited in memory, or for very large, highly resolved simulations. A Cartesian system, by comparison, can account for asymmetry in the laser beam shape, and allows more complicated geometries (such as beams close to an edge). Additionally, in such a Cartesian system, photon collection “bins” are all of a uniform size, making data consistent as the horizontal distance from the light source increases.
3.1.2 Photon Positioning and Initial Conditions

The term “photons” used in this simulation is not directly equivalent to the photons found in particle physics. In this study, “photon” is used to represent a conceptual unit of light in the simulation. In each simulation, the number of photons run is $N_{\text{photons}}$. Larger values of $N_{\text{photons}}$ decreases random variations in the distribution obtained at the expense of the prolonged computation time. Typically, between $10^4$ and $10^5$ photons are run. Each photon in the simulation is assigned a “weight”, $w$, of unity. As the photon propagates through the medium, it slowly loses weight at each scattering event. To prevent photons from continuing indefinitely, the photon is removed when its weight falls below a certain threshold.
Each photon is positioned with the same initial position at the top surface of the block, denoted by $x$, $y$ and $z$,

$$x_{\text{initial}} = \frac{x_0}{2}$$

$$y_{\text{initial}} = \frac{y_0}{2}$$

$$z_{\text{initial}} = 0$$

The cosines of the angles the photon trajectory makes with each Cartesian axis, $u_x$, $u_y$ and $u_z$, are used to determine the photon’s next position. For this simulation, each photon is assumed to have the same initial direction, normal to the incident surface.

$$u_x = 0$$

$$u_y = 0$$

$$u_z = 1$$

### 3.1.3 Photon Step

Propagation of the photon through the material is next addressed. To move through the material, the photon takes a step along the direction it is currently traveling. Initially, it steps along $z$ (as determined in Equation (11). Wilson et al. [9] selected the step size to be random such that

$$\text{step} = \frac{-\ln(\xi)}{\mu_k}$$

$\xi$ denotes a uniform random number on $[0,1]$, while $\mu_k$ is the extinction coefficient. This coefficient, as discussed in 2.1.1, is the sum of the absorption ($\mu_a$) and scattering ($\mu_s$) coefficients. Over many steps, the average step size is $\frac{1}{\mu_k}$ and is defined as the mean free path length [34].
Random numbers with a normal distribution are generally not desirable due to their sampling bias; in normal distributions, values in the middle of the range are more probable than those at the limits. Using a uniform distribution, it can be shown that the mean-free path length, or the average step size, is simply the inverse of the extinction coefficient, $\mu_k$. In this laser propagation model, MATLAB’s built-in pseudorandom number generator “rand()” is used.

With a step size chosen, the photon’s position is updated accordingly:

\[
\begin{align*}
    x_{\text{new}} &= x_{\text{old}} + ux \times \text{step} \\
    y_{\text{new}} &= y_{\text{old}} + uy \times \text{step} \\
    z_{\text{new}} &= z_{\text{old}} + uz \times \text{step}
\end{align*}
\] (13)

As the direction of the photon has not yet been updated from the initial condition, the first step, though of variable length, is always normal to the XY plane, along Z into the material.

### 3.1.4 Photon Absorption

At the end of each step, there is some absorption of the photon’s weight at its new location, meant to simulate local heating in the material. As the material is subdivided into a succession of bins, the photon’s current bin is located within the absorption matrix $Q$. Wilson [9] used Equation (14), below, to describe the fraction of the photon’s current weight that is lost at each step:

\[
Q(i, j, k) = Q(i, j, k) \times w\left(\frac{\mu_a}{\mu_k}\right)
\] (14)

Here, $i, j$ and $k$ represent the bin indices corresponding to the bin containing the photon’s current position, $(x, y, z)$ and $\mu_a$ is the absorption coefficient. The photon’s remaining weight is given by:

\[
w_{\text{new}} = w_{\text{old}} \left(1 - \frac{\mu_a}{\mu_k}\right) = w_{\text{old}} \left(\frac{\mu_s}{\mu_k}\right)
\] (15)
3.1.5 Photon Scatter

After a partial absorption event, the photon direction changes, due to scattering off crystals or fibres within the part. As the program works in three dimensions, an azimuthal angle $\phi$, in the X-Y plane, and a deflection angle $\theta$, along Z, are chosen (Figure 3-3). The azimuthal direction is chosen to lie with equal probability on $[0,2\pi]$, as scattered radiation is assumed to be unpolarized [15]. That is,

$$\phi = \xi' \times 2\pi$$

(16)

where $\xi'$ is a new, uniform random number.

![Figure 3-3 Coordinate system showing azimuthal and deflection angle definitions](image)

The deflection angle $\theta$, which defines forward (or backward) scattering is slightly more complicated. Use of Mie Theory, the solutions of Maxwell’s equations for scattering off spherical particles, was considered. However, determining a phase angle using the Mie solutions is neither trivial [36] nor is it simple to account for the various sizes and shapes of particles that might exist in a single material, given that spherulites, pigments, fillers and fibres and other particles are all materials off which scattering may occur. An approximation to Mie’s analytical solution comes in the form of the Henyey-Greenstein (HG)
function [32]. This function is used here as an approximate solution to the “phase problem”. The HG phase function is rearranged to provide the deflection angle [34] as

$$\theta = \arccos \left( \frac{1 + g^2 - \left(1 - g^2 \right)^2}{2g} \right)$$

where $\zeta$ is a uniform random number and $g$ is the anisotropy factor, the third of the four user-specified model parameters.

Provided with an azimuthal and deflection angle, the photons trajectory is updated before the next step is calculated. Ilie et al. [15] calculated these using:

$$u_{x_{new}} = \frac{\sin(\theta)(ux_{old}ux_{old} \cos(\varphi) - uy_{old} \sin(\varphi))}{\sqrt{1 - uz_{old}^2}} + ux_{old} \cos(\theta)$$

$$u_{y_{new}} = \frac{\sin(\theta)(uy_{old}ux_{old} \cos(\varphi) - ux_{old} \sin(\varphi))}{\sqrt{1 - uz_{old}^2}} + uy_{old} \cos(\theta)$$

$$u_{z_{new}} = -\sin(\theta) \cos(\varphi) \sqrt{1 - uz_{old}^2} + uz_{old} \cos(\theta)$$

In the unique case where $uz \cong \pm 1$, the denominator of the $ux$ and $uy$ direction cosines becomes zero. As Ilie [15] showed, the new direction cosines can be calculated using:

$$u_{x_{new}} = \sin(\theta) \cos(\varphi)$$

$$u_{y_{new}} = \cos(\theta) \sin(\varphi)$$

$$u_{z_{new}} = uz_{old} \cos(\varphi)$$

### 3.1.6 Photon at a Boundary

Due to a change in the index of refraction at boundaries, real-world rays of light exhibit either splitting, where the ray is partially reflected and transmitted, or pure reflection. Analogously, in this simulation,
photons may be both reflected and transmitted, or totally internally reflected, depending on their approach angle. The simulation assumes that, at every boundary, air is the external medium, with a constant index of refraction of unity.

At every step, the photon’s position is checked to verify that it has not exceeded the specified X, Y and Z limits. If any limit is exceeded, the photon returns to its previous position. For the case of a photon exceeding the YZ boundary, for example:

\[ x_{\text{new}} = x_{\text{current}} - ux \times \text{step} \]

\[ y_{\text{new}} = y_{\text{current}} - uy \times \text{step} \]  
(20)

\[ z_{\text{new}} = z_{\text{current}} - uz \times \text{step} \]

With the photon at its previous position, the exact size of a step to the boundary along the current direction is calculated. Continuing with the case of a photon approaching the YZ boundary:

\[ \text{step}_{\text{boundary}} = \left| \frac{x_{\text{new}}}{ux} \right| \]  
(21)

The position is updated to bring the photon exactly to the boundary.

\[ x_{\text{boundary}} = x_{\text{current}} + ux \times \text{step}_{\text{boundary}} \]

\[ y_{\text{boundary}} = y_{\text{current}} + uy \times \text{step}_{\text{boundary}} \]  
(22)

\[ z_{\text{boundary}} = z_{\text{current}} + uz \times \text{step}_{\text{boundary}} \]

Note that, in this case, \( x_{\text{boundary}} = X_0 \). Next, the program must decide how the photon proceeds; either, there is a case of total internal reflection and all of the photon is returned to the medium, or some portion of the photon’s weight escapes. Perfect transmission due to Brewster’s angle is not considered.
3.1.6.1 Total Internal Reflection

Total internal reflection occurs when light hitting the interface is shallow enough that the angle of incidence, $\theta_i$, is greater than the critical angle, $\theta_c$. In this case, with light attempting to leave the material, the critical angle is

$$\theta_c = \arcsin\left(\frac{n_2}{n_1}\right)$$

(23)

where $n_2$ is the refractive index of air, and $n_1$ that of the material, the last of the four user-specified model parameters. If the incident angle is greater than this critical angle, no photon weight is changed. Rather, the direction is reversed, simply by switching the sign of the appropriate directional cosine. Continuing with the case of a photon reflected off the YZ interface,

$$x_{\text{new}} = x_{\text{boundary}} + (-ux) \times (\text{step} - \text{step}_{\text{boundary}})$$

$$y_{\text{new}} = y_{\text{boundary}} + uy \times (\text{step} - \text{step}_{\text{boundary}})$$

(24)

$$z_{\text{new}} = z_{\text{boundary}} + uz \times (\text{step} - \text{step}_{\text{boundary}})$$

Thus the photon continues along with this reversed direction for the remainder of the originally calculated step.

3.1.6.2 Partial Reflection

If the angle is less than the critical angle, part of the ray is transmitted and the remainder reflected. The simulation models this by splitting the weight of the photon, and recording the escaped portion in the appropriate two dimensional “face” matrix, as discussed in Section 3.1.1.

The portion reflected, $R$, is determined by the Fresnel reflection coefficients, while the transmission, $T$, is simply the difference between $R$ and unity. Having scattered through the medium, the light is considered to be unpolarized [15], so reflection coefficients for both $p$-polarized and $s$-polarized light are computed [37], and their mean value utilized according to
The photon’s weight is next updated, and the escaped weight is recorded in the required face matrix. Continuing with an example of a photon at the YZ boundary,

\[ R_p = \left| \frac{n_1 \cos(\theta_2) - n_2 \cos(\theta_1)}{n_1 \cos(\theta_2) + n_2 \cos(\theta_1)} \right|^2 \]  
\[ R_s = \left| \frac{n_1 \cos(\theta_1) - n_2 \cos(\theta_2)}{n_1 \cos(\theta_1) + n_2 \cos(\theta_2)} \right|^2 \]  
\[ R = \frac{R_p + R_s}{2} \]  
\[ T = 1 - R \]  

This way, a complete description of the weight escaped and its distribution are recorded in the face matrices. The reflected photon continues along its original step with a reversed direction cosine, as described above in section 3.1.6.1.

### 3.1.7 Photon Death

As the photon’s weight decreases, either by transmission at the interface or absorption, any remaining events are of diminishing value as there is less weight to be deposited at each step. Additionally, it is computationally impossible to continually track the photon’s weight down to 0, as a fraction and not an absolute amount of the remaining weight is removed with each interaction. Therefore, an approximation must be used. Here, the photon weight threshold, \( w_t \), is utilized, typically chosen to be \( 10^{-4} \). Once the photon’s weight falls below this threshold, it is removed and a new photon launched.

There is a problem with this, however. While each photon begins with a weight of 1, the cumulative weight left by that photon in the absorption and face matrices can only ever sum to the value of one minus the threshold. In order to conserve universal photon weight, then, a game of chance is implemented [34].
Photons whose weight falls below the threshold are “killed”, but are given the chance of being reincarnated with a new weight. A chance of $1/10$ is chosen for this simulation, and successful photons are reborn with ten times their under-threshold weight. This way, every tenth photon (on average) makes up the remaining weight and the total is preserved. The value of $1/N_{\text{photons}}$ should always be significantly smaller than the chance chosen, to preserve the average and thus the statistical likelihood of a fair game.
3.2 Adapting the Monte Carlo Method to Specific Laser Beam Profiles

The simulation described in the previous section is that of a single photon originating from a lone point source located on a volume with fixed optical parameters. In practice, few lasers are ideal point sources of light. Furthermore, not all lasers have straightforward, mathematically defined profiles (Gaussians, Top-Hat distributions etc.). In the case of the Rofin laser system used in this research, the profile is both asymmetrical in X and Y and its distribution can vary significantly over a range of few millimeters above and below the focal plane, as shown in Figure 3-4 and Figure 3-5, below.

![Figure 3-4 Two-dimensional beam profile for the Rofin laser system, in focus](image-url)
It is therefore necessary to adapt the Monte Carlo simulation described above to be able to predict the transmitted distribution, transmission and reflection for a variety of incoming laser beam profiles.

3.2.1 Initialization
With the Monte Carlo method completed, the absorption matrix $Q$ and the “face” matrices are saved. The next portion involves a technique for scaling these results according to a given beam profile. The master matrix, “$M$”, which will contain the final three-dimensional absorption data is defined. Master matrices for each of the two-dimensional face matrices - $M_X$, $M_X0$, $M_Y$, $M_Y0$, $M_Z$ and $M_Z0$ – are also set up. These matrices will be used to store the scaled distributions of escaped photon weights.

3.2.2 Matching Beam Profile Data to Simulation Resolution
The incoming laser beam profile can be obtained by pinhole measurements of beam intensity for given X-Y location data [17]. This data, consists of X and Y location data, and the beam intensity at each location.
Next, a new scaling array, $S$, is constructed to house the beam profile. The imported beam profile data is used to set a scale for $S$; the total $X$ and $Y$ dimensions of the beam profile are divided by the $\Delta x$ and $\Delta y$ resolutions used in the Monte Carlo method previously. That is,

$$\dim(S) = \left[\frac{X_{beamdata}}{\Delta x}, \frac{Y_{beamdata}}{\Delta y}\right]$$

(31)

If $X_{beamdata}$ or $Y_{beamdata}$ are not wholly divisible by $\Delta x$ and $\Delta y$ respectively, an extra bin is added to account for the remainder.

The original beam profile data is interpolated to provide values for each element of $S$. The MATLAB interpolation function, griddata is used for this, using a linear interpolation between successive beam profile points. In this way, $S$ is constructed to match the resolution of the original Monte Carlo simulation. The original beam profile and a sample $S$ are shown side by side in Figure 3-6.

![Fig 3-6](image)

**Figure 3-6** Original beam profile data, left, and $S$, the interpolated data matching the resolution used in the Monte Carlo simulation
3.2.3 Filling the Master Matrices

With the beam profile matching the resolution of the original simulation, the next step is to scale the original simulation data according to the distribution set out by the beam profile.

Each non-zero location on the beam profile, S, is used as a scaling multiplier for the entire absorption matrix Q, and the face matrices. Each element of these matrices is multiplied by each non-zero location on S and added to the respective master matrix, creating a superposition. Mathematically, for the Z master matrix:

$$M_{Z_{xy}}[i,j] = \sum_{j=1}^{N_x} \sum_{i=1}^{N_y} S_{xy} * FZ[i,j]$$

where $S_{xy}$ is a non-zero location on the unscattered beam profile S. The calculation is repeated for every value of S. In this way, a complete description of the overall beam profile distribution after scattering is created by taking the distribution for a single point source beam, centering it at each discrete location of the unscattered beam profile, and scaling by the value of the beam at that point. The overlapping image produced is the complete description of the Monte Carlo method for the beam profile used.

Figure 3-7 demonstrates this concept in the case of the Z face matrix, $FZ$. This matrix records photons escaping through the weld interface. The figure shows an extreme case where the incoming laser beam profile is only defined in four places. The FZ master matrix, $MZ$ is calculated by adding four scaled versions of the original $FZ$ matrix.
Figure 3-7 Filling the MZ master matrix by scaling point source data, according to the values of the beam profile “S”
3.3 Summary

The simulation consists of a Monte Carlo simulation, and a scaling algorithm to recreate the Monte Carlo data according to a specific incoming beam profile.

The Monte Carlo relies on four primary optical parameters:

- **Scattering Coefficient, $\mu_s$** – Makes up part of the extinction coefficient, which determines the average step size of each photon and thus the average number of steps for which a photon remains in the material. Measured in mm$^{-1}$.

- **Absorption Coefficient, $\mu_a$** – How absorptive the material is to light at this wavelength. Affects the size of the fraction of light absorbed at each step. Makes up part of the extinction coefficient, along with $\mu_s$. Measured in mm$^{-1}$.

- **Anisotropy Factor, $g$** – Helps determine the next direction a photon will travel in after a scattering event. Determines how forward (or backward) directed scattering is. Unitless. Can range between -1 and 1. A value of +1 indicates that the photon direction never changes, while a value of 0 indicates that scattering is totally isotropic.

- **Refractive Index, $n$** – The refractive index. Determines the portion of weight of a photon that may escape the material at an interface, as a function of its incident angle.

Additionally, the dimensions of the part, $X$ and $Y$, as well as thickness, $Z$, are required. The number of photons simulated $N_{\text{photons}}$, and the resolutions $\Delta x$, $\Delta y$ and $\Delta z$ are also necessary.

The Monte Carlo results are then scaled according to the incoming beam profile, to emulate the scattered distribution that would result from such a profile.

The code for the laser propagation model is listed in Appendix A.
Chapter 4. Simulation Validation and Behaviour

As discussed in Section 2.3, the simulation was coded entirely in the MATLAB programming language.

The simulation was tested for consistency in two ways. First, all photons had to be accounted for. Second, the program’s adherence to the common law of absorption, Beer’s Law [38], was examined.

The number of photons necessary to achieve a statistically similar result over several trials was also determined. The effect of bin size – the resolution - on the simulation precision, runtime and memory was also examined. Finally, the effect of tuning the four optical parameters – anisotropy, refractive index and the scattering and absorption coefficients – was assessed.

4.1 Balancing the Photon Count – Conserving Photon Weight

In this Monte Carlo technique, all the photons transported through the material need to be accounted for. Therefore, the total weight of photons in must be equal to the total weight of photons collected in the Q absorption matrix, and the six face matrices. Mathematically,

\[ N_{\text{photons}}w_{\text{photon}} = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} (Q_{ijk} + FX_{ijk} + FX0_{ijk} + FY_{ijk} + FY0_{ijk} + FZ_{ij} + FZ0_{ij}) \]  

The initial photon weight used was always unity, and the resolution \( N_x, N_y, N_z \) was determined previously in Equation (9). For this photon counting exercise, the other simulation parameters were chosen at random for each of the trials, to identify any irregularities in the input/output. Table 4-1 gives these results.

<table>
<thead>
<tr>
<th>Photon Weight In (N\text{photons})</th>
<th>Photon Weight Out (Trial 1)</th>
<th>Photon Weight Out (Trial 2)</th>
<th>Photon Weight Out (Trial 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>99.99786</td>
<td>100.0007</td>
<td>99.99998</td>
</tr>
<tr>
<td>1000</td>
<td>999.9703</td>
<td>999.9463</td>
<td>999.9722</td>
</tr>
<tr>
<td>10000</td>
<td>9999.728</td>
<td>9999.619</td>
<td>9999.500</td>
</tr>
<tr>
<td>100000</td>
<td>99996.46</td>
<td>99996.30</td>
<td>99996.56</td>
</tr>
</tbody>
</table>
There is very little difference between the total weight in and weight out in each trial; the discrepancy between numbers is assumed to be due to round-off error during the simulation.

4.2 Examination of Beer’s Law

The Beer-Lambert-Bouguer Law, as discussed in 2.1.1, describes the absorption of light as a function of the depth through a material, so long as the material is non-scattering.

To confirm that the simulation accurately models light behaviour, total photon weights absorbed in the Q-matrix for a given depth should be predicted by the exponential decay for the same absorption coefficient. Therefore, comparing the results must be done along a single axis - photon weight against depth. To examine all of the photon weights at a given depth, the entire slice of Q is summed along the X and Y directions, for each depth:

\[
W(z)_{\text{Simulation}} = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} Q_{ij}(z)
\]  

(34)

Q is an \(N_x\) by \(N_y\) by \(N_z\) matrix. Therefore summation along the \(x\) and \(y\) dimensions yields a single value, representing the total photon weight for a single “slice”. These summations, at each \(Z\), make up a column of photon weights as a function of depth.

In choosing optical parameters for the examination of Beer’s Law, a non-scattering case is required. Recalling that \(g\), the anisotropy factor, is an average measure the forward- or backward-directed scattering in the material, a value of unity is chosen; in other words, the photon direction never changes from the initial setting, of \(uz = I\). The primary contribution of the scattering coefficient, \(\mu_s\), is in the determination of the step size, which is related to the average lifetime of a photon within the material. Therefore, changing this is likely to have an effect on the number of photons required for a statistically significant result. For consistency, a constant value of unity is used. An index of refraction typical of amorphous polymers of 1.6 was used. Geometrically, a simple cube was specified, with \(X_0 = Y_0 = Z_0 = 10\text{mm}\) with a resolution of 10\(\mu\text{m}\), corresponding to a total of 1000 bins along the \(Z\) direction.
Several simulations were run, ignoring any specific laser beam power intensity profiles and instead using only a single point source. Figure 4-1 shows the results for several absorption coefficients, each with the corresponding analytical Beer’s Law function plotted in black. The code “C32” appearing to the top-right of the figure refers to the MATLAB script used to generate the figure.

![Figure 4-1 Simulation of Beer's law behaviour for varying absorption coefficients](image)

In each simulation, the analytical Beer’s Law function is in good agreement ($R^2>0.98$) with the simulation data for each absorption coefficient used. These results indicate that the simulation can estimate absorption within the material in non-scattering cases. Close examination of the data around the surfaces, at $z = 0\text{mm}$ and $z = 10\text{mm}$ shows tendencies of the simulation data to be higher than the analytical function. This is thought to be due to internal reflection at boundaries, something the simulation accounts for but Beer’s Law does not.
4.3 Determining the Iteration Count Necessary

The number of photons, $N_{\text{photons}}$, necessary to achieve a repeatable result must be considered. Depending on the measure, the number of iterations necessary for reproducible results can vary – variations in anisotropy, scattering and absorption coefficients, the dimensions of the simulated block and even the photon death threshold may affect the outcome. As an example, one might take the situation where the light distribution at the weld interface is examined. A simulation with low anisotropy ($g<<1$) means that photons’ scattering is less forward directed than anisotropy factors closer to unity. As a result, less photon weight reaches the interface, and more photons are necessary to achieve a significant accumulation at the MZ face matrix. Conversely, application of a beam profile, rather than a point source, improves the repeatability of a simulation at lower photon counts. This is due to the program’s addition of a single Monte Carlo simulation over each resolved point of the beam profile (Section 3.2), rather than conducting a separate, weighted simulation at each point of the beam profile – a trade-off for speed. Aberrations may be minimized during this summation procedure.

Therefore, although it appears that there is no single solution for the number of photons required for a reproducible distribution, determination of the necessary value of $N_{\text{photons}}$ for a single given simulation is possible. As the program was originally developed to compare distributions at the weld interface with experimentally measured distributions, the distribution at the master Z face matrix, the $MZ$ matrix, are used.

4.3.1 Calculating the T-NPFD

As discussed, the beam profile may not be symmetrical about any axis. The primary scanning direction is taken to be along the X direction. Figure 4-2 shows the cumulative weight of photons recorded on the $MZ$ matrix. These are the photons escaping the transparent part at the weld interface. As the beam scans in the X direction, the total photon weight for a given value of Y is summed to provide a complete transverse beam profile, referred to as the transverse power flux distribution, or T-PFD.
The colour plot represents the number of photons accumulated on the X-Y plane at the weld interface for a Gaussian beam after passing through a relatively low-scattering material. Mathematically, for each bin $j$, the value of the T-PFD is given as:

$$TPFD_j = \sum_{i=1}^{N_x} MZ_{ij}$$  \hspace{1cm} (35)

As Zak et al. [11] showed, the transverse normalized power flux distribution (T-NPFD) is given by scaling the distribution so that the area under the curve is equal to unity as shown in Equation (4). For a finite number of bins, the integral becomes a summation, with each element of the T-NPFD given by:

$$TNPFD_j = \frac{TPFD_j}{\sum_{j=1}^{N_y} TPFD_j dy}$$  \hspace{1cm} (36)

By normalizing, the distribution is consistent regardless of the number of photons used.
As the number of photons used increases, the more repeatable the result becomes, though as Figure 4-3 shows, computation time increases linearly with the number of photons used. Though the size of $N_{\text{photons}}$ has the largest impact on runtime, changing other parameters, such as the scattering (Figure 4-3), have a somewhat smaller influence, as shown.

![Figure 4-3 Effect of scattering coefficient and photon count on simulation runtime](image)

As the average step size is the inverse of the extinction coefficient $\mu_k$, as discussed in Section 3.1.3, and $\mu_k = \mu_a + \mu_s$, an increase in the scattering coefficient leads to a smaller value of $\frac{1}{\mu_k}$, resulting in photons taking a greater average number of steps within the material. As they must undergo more interactions, processing time is increased. To minimize the number of photons necessary for a simulation, the difference between simulations with identical values of $N_{\text{photons}}$ is measured objectively.

This objective value is calculated as:

$$A_{\text{rss}} = (TNPFD - TNPFD^*)^2$$

(37)
where *TNPFD* is the transverse normalized power flux distribution for the first trial. TNPFD*, is the transverse normalized power flux distribution calculated for the second trial with the same value of \(N_{\text{photons}}\). The value \(A_{\text{rss}}\) is a real number that gives a raw measure of how similar these two distributions are. A smaller value indicates a result with less variability.

It is expected that as \(N_{\text{photons}}\) grows, the value of \(A_{\text{rss}}\) continually shrinks in the limit

\[
\lim_{N_{\text{photons}} \to \infty} A_{\text{rss}} = 0
\]  

Figure 4-4, next, shows the effect of increasing the number of photons on \(A_{\text{rss}}\). Each point was obtained by calculating the objective difference between the T-NPFDs obtained for successive identical simulations, with arbitrary optical parameters.

![Figure 4-4 Effect of photon count on sequential value of \(A_{\text{rss}}\)](image)

As expected, increasing the number of photons reduces the variation in successive runs. It was determined that for calculating T-NPFDs, \(10^4\) photons was sufficient. To verify the appearance of the distribution at
some of these values, Figure 4-5 gives the T-NPFDs for increasing $N_{\text{photons}}$ in a 3mm thick sample, using point source of light with arbitrary optical parameters.

![Figure 4-5 T-NPFD for a point source beam, multiple values of $N_{\text{photons}}$](image)

$10^2$ photons, with a corresponding $A_{rs} \approx 80$, it is difficult to recognize as a beam profile. At $N_{\text{photons}} = 10^3$, the objective difference between successive simulations is less than 10 and a T-NPFD is apparent. At $10^4$, with $A_{rs} < 1$, there is virtually no difference between simulations with increased photon counts. Here, $N_{\text{photons}}=10^5$ was judged to be acceptable.
4.4 Selecting a Resolution

Resolution of the simulation is, along with the number of photons fired, the major factor affecting simulation runtime – therefore, an acceptable resolution must be selected for speed. Specifically, the resolution is determined by the number of bins, and thus the ratios of $N_i$ to $Ax$, etc.

The first part of the simulation is a Monte Carlo procedure that utilizes a single point source of light to determine photon paths. As Figure 4-6 shows, this component is unaffected by resolution. To understand why this is the case, recall that the simulation relies on a three dimensional absorption matrix, $Q$, that is subdivided into a number of bins, each with a finite volume $AxAyAz$. At each step, photons are partially absorbed. The location is recorded simply by locating the bin the photon currently occupies and updating the value of the weight in that bin. Therefore, the number of bins should not have any effect on the rate at which this procedure takes place. Instead, as Figure 4-3 showed, it is primarily the number of photons used that determines this runtime.

Conversely, the execution speed of the second component is unaffected by the number of photons fired and instead is solely a function of the resolution of the simulation. This component utilizes a completed simulation. The absorption matrices are scaled and added repeatedly to a single corresponding master matrix, as discussed in Section 3.2. More bins require more calculations, and as a result, longer processing times.

To summarize; the key determinant in the Monte Carlo simulation is the number of photons fired, while the resolution primarily affects the adaptation of the simulation to a specific beam profile.

Additionally, one may note that while increasing the number of photons used in a single simulation increases the time required linearly (Figure 4-3), increasing the resolution can mean increasing the number of calculations – and thus time required - by exponential factors, as shown in Figure 4-6.
Choosing a resolution, for the simulation, therefore, becomes a problem of time and necessity. If, for example, experimental data can only be obtained at 300μm spacing, for the purpose of data matching, it makes little sense to utilize more memory and time-intensive resolutions. Like the number of photons necessary, the resolution required needs to be evaluated on a case-by-case basis.
4.5 Exploring the Effect of Refraction, Anisotropy, Scattering and Absorption

The effect of material optical parameters on photon behaviour was examined. The influences of anisotropy, absorption and scattering coefficients and the index of refraction are assessed here. As in previous sections, the T-NPFD in the X-direction at the weld interface, as well as transmission, is used to examine these parameters.

Each of the optical parameters examined here are assumed to be constant for the purpose of this model. In reality, they are expected to vary slightly with temperature and changes in phase at the weld interface.

The number of photons used, resolution, part size and incoming beam profile are all kept constant (Table 4-2). The optical parameters are also held constant, except where otherwise indicated. A depth of 3 mm is typical of laser welded plaques.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Photons</td>
<td>10000</td>
<td>-</td>
</tr>
<tr>
<td>Bin Size</td>
<td>0.2</td>
<td>Millimeters</td>
</tr>
<tr>
<td>Part X-Dimension</td>
<td>10</td>
<td>Centimeters</td>
</tr>
<tr>
<td>Part Y-Dimension</td>
<td>10</td>
<td>Centimeters</td>
</tr>
<tr>
<td>Part Z-Dimension</td>
<td>3</td>
<td>Centimeters</td>
</tr>
<tr>
<td>Absorption Coefficient, $\mu_a$</td>
<td>0.2</td>
<td>1/Millimeters</td>
</tr>
<tr>
<td>Scattering Coefficient, $\mu_s$</td>
<td>2</td>
<td>1/Millimeters</td>
</tr>
<tr>
<td>Anisotropy Factor, g</td>
<td>0.8</td>
<td>-</td>
</tr>
<tr>
<td>Index of Refraction, n</td>
<td>1.6</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 4-2 Simulation parameters used in each trial

Each optical parameter is tested across its full range of expected variability. In each case, both a point source and the in-focus Rofin laser beam profile measured by Mayboudi [17] are used.
4.5.1 Anisotropy
To observe the effect of anisotropy, the exit beam profile is examined in the scanning direction. Figure 4-7 and Figure 4-8 show the T-NPFDs for three values of $g$, taken across the positive range of the variable. Although $g$ can range between -1 and +1, negative values of $g$ are not considered as it is assumed materials with high degrees of backscattering are unsuitable for laser welding.

![Figure 4-7 T-NPFD for a point source of light as a function of $g$](image-url)
Figure 4-8 T-NPFD for an in-focus Rofin laser as a function of $g$

Higher values of $g$ provide a narrower distribution that scatters relatively little as it traverses the 3mm thick part. With lower values of $g$, there is greater beam divergence, as expected. As discussed in 4.3, localized fluctuations are reduced after the weighted summation procedure, despite the significant amount displayed by the curves in Figure 4-7.

Transmission was calculated as the ratio of photons absorbed in the $MZ$ matrix to the total number of photons initially fired. Figure 4-9 gives the corresponding transmission numbers for several values of $g$. 

46
4.5.1 Transmission

For forward directed scattering (high values of $g$) transmission rates are higher, as photons are less likely to be greatly scattered away from their original heading along the Z-axis into the material. As a result, more photons make it through the material and exit at the weld interface. In the unique case where $g=1.0$, the transmission is very close to the value predicted by the Beer-Lambert equation for the same absorption coefficient, with a 3% difference in prediction. The discrepancy here might be explained by recognizing that while the simulation takes into account internal reflection, the Beer-Lambert relationship does not, as it is only meant to provide a decay distribution for a boundaryless continuous material.

4.5.2 Scattering

The scattering coefficient, $\mu_s$, makes up part of the extinction coefficient, $\mu_k$, which determines the average step size and thus the frequency of laser-material interactions. Figure 4-10 and Figure 4-11 show the T-NPFDs for a point source and the in-focus ROFIN laser respectively.
Figure 4-10 T-NPFD for a point source as a function of $\mu_s$.

Figure 4-11 T-NPFD for an in-focus Rofin laser as a function of $\mu_s$. 

48
Like anisotropy, changes in the scattering coefficient appear to affect the dispersion significantly, though not as dramatically as large scale changes to $g$. Higher values of $\mu_s$ decrease the average step size and thus increase the number of times a photon is likely to scatter. As each distribution is normalized, distributions with longer tails result in a lower overall peak height, as the normalization procedure calculates the total area under the graph. Figure 4-11 shows that increasing the coefficient from 1 mm$^{-1}$ to 2 mm$^{-1}$ results in a change to peak height of almost 40%, indicating higher degrees of scattering.

Transmission for several values of $\mu_s$ was examined. Figure 4-12 shows transmission values for a wider range of scattering coefficients.

![Graph showing transmission as a function of $\mu_s$](image)

**Figure 4-12 Transmission as a function of $\mu_s$**

As expected, low scattering coefficient values result in higher transmission. For low values each photon is scattered less often on its path through the material, it deposits less energy overall, resulting in a higher proportion of its energy available at the weld interface.
4.5.3 Absorption

The effect of absorption on the exit beam T-NPFD is observed here. Three values of the parameter are chosen and distributions are presented for a single point source beam (Figure 4-13) and for the in-focus Rofin laser [17] (Figure 4-14).

![Figure 4-13 T-NPFD for a point source as a function of $\mu_a$](image-url)
Figure 4-14 T-NPFD for an in-focus Rofin laser as a function of \( \mu_a \)

With the point-source distribution, the absorption has little effect on the shape of the beam profile. For the actual beam profile (Figure 4-14), tripling the absorption results in a change to the peak height of less than 20\%, indicating relatively little scatter.

Transmission data in for a greater range of \( \mu_a \) is shown in Figure 4-15.
While the distribution is not affected greatly by the absorption coefficient, it has a significant effect on the transmission. For example, doubling its value from 0.1 mm$^{-1}$ to 0.2 mm$^{-1}$ reduces the transmission from 23% to 15%. This suggests that a decoupling of variables can be employed during model parameter estimation – scattering and anisotropy variables may be used initially to match an experimental beam profile, while the absorption parameter is individually adjusted to match the corresponding experimentally estimated laser transmission.

4.5.4 Refraction
The index of refraction is the final parameter examined. This index is generally accepted to lie between 1.2 and 1.6 for most plastics at 20°C, with a limited wavelength dependency in the 500-1500nm range. Polycarbonate, for example, is around 1.58 [39], while polyamide-6 is around 1.50 [40].

Four indices of refraction were simulated and the results displayed in Figure 4-16. The boundary was assumed to be air, with a corresponding index of refraction of $n_{\text{air}} = 1$. 

![Figure 4-15 Transmission as a function of $\mu_a$](image)
The figure shows the effect of the material index of refraction on the T-NPFD. It can be seen that as index of refraction of the material gets closer to the index of refraction in air, the peak height decreases, indicating higher scattering. This might be explained by consideration of the critical angle (Section 3.1.6.1). As \( n_{\text{mat}} \) increases, the critical angle decreases, and only photons with smaller angles of incidence can be transmitted. As the horizontal distance from the laser source increases, the angle of incidence of a photon is likely to be higher. A higher incident angle makes it more likely to be totally internally reflected, especially if the critical angle is also small. Thus, internally reflected photons cannot contribute to the exit beam profile, resulting in the less scattered distribution seen at the interface. Conversely, as \( n_{\text{mat}} \rightarrow n_{\text{air}} \), a larger critical angle means that photons can be transmitted at more angles, resulting in more transmission further from the source, and thus more scattering. Change to the overall shape of the T-NPFD, is small, with a 60% change to \( n_{\text{mat}} \) resulting in only a 10% change to the peak height.

Figure 4-16 T-NPFD for an in-focus Rofin laser as a function of \( n_{\text{mat}} \)
Transmission data is shown below in Figure 4-17. Like the exit beam profile, major changes to the index of refraction result in small changes to the transmission.

Figure 4-17 Index of Refraction versus Transmission

Figure 4-17 shows a linear relationship between refraction and transmission. As $n_{\text{mat}} \to n_{\text{air}}$, transmission increases to approximately 25% when the material index is matched to the index of air as expected. Compared to anisotropy, scattering and absorption, the effect of $n_{\text{mat}}$ on transmission is relatively small.
Chapter 5. Estimating Model Parameters from Experimental Data

Although the simulation produces reasonable results, there is no clear idea of what optical parameters might be required to accurately reproduce transmission, reflection or T-NPFD data for a new material. The index of refraction aside, without further testing, the settings of the other three Monte Carlo optical parameters (\(g\), \(\mu_o\), \(\mu_a\)) remain unknown. This chapter discusses the technique employed in establishing the likely values for each of these variables in specific materials.

5.1 Equipment and Materials

The laser system used to gather the experimental data in this project is a Rofin DL x16 Industrial Diode laser, operating at a wavelength of 940nm, with a power over the range 10 – 160W. The system is mounted in an enclosure which is located in Jackson Hall, on the Queen’s University campus. The DL x 16 systems nominally focuses with a spot size of 0.6mm \(\times\) 1.4mm at a working distance of 83mm [41].

Data on the two dimensional beam profile of this Rofin laser for use in the beam scaling algorithm discussed in Section 3.2 was obtained from the work done by Mayboudi in 2006 [17].

The experimental T-NPFD and transmission data used was gathered by Xin Feng Xu, a post-doctoral fellow at the Royal Military College. For each material, plates were prepared by injection moulding on an Engel 55 ton injection moulding machine located at RMC. To produce a T-NPFD of a beam transmitted through a transparent plate, the line-scanning technique proposed by Zak et al. [11] was used. Laser-scanned lines were generated on a polyamide-6 (PA6) sample polymer containing 0.2% carbon black supplied by DSM by placing it below the transparent plate at a working distance of 82.5mm. Using a scanning speed of 2000mm/min, the laser power was incrementally ramped to generate lines of increasing width. A series of these lines is shown in Figure 5-1.
Figure 5-1 Laser scan lines produced on the sensor polymer using a 2.2mm PA6-20%LGF sample as the top part

Transmission values were measured using the technique developed by Azhikannickal et al. [21]. An injection moulded plate was placed directly on a Coherent PowerMax PM10 portable power meter, positioned at 90° to the incident laser beam. The incident laser power with and without the plate was then measured. The accuracy on these measurements was specified as ±5%.

Both amorphous and semi-crystalline thermoplastics were examined. Glass fiber filled polycarbonate samples were provided by Osterman, a company specializing in distributing thermoplastics [42]. Table 5-1, below, summarizes the glass fibre concentrations for each of the PC samples provided.

<table>
<thead>
<tr>
<th>Material</th>
<th>Osterman Trade Name</th>
<th>Glass Fibre Content (% GF)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PC10GF</td>
<td>PC950G</td>
<td>10.8</td>
</tr>
<tr>
<td>PC15GF</td>
<td>PC952G</td>
<td>16.7</td>
</tr>
<tr>
<td>PC30GF</td>
<td>PC953G</td>
<td>31.8</td>
</tr>
<tr>
<td>PC40GF</td>
<td>PC954G</td>
<td>40.7</td>
</tr>
</tbody>
</table>
For each of these PC materials, the transmission data and a T-NPFD were recorded for plates of multiple thicknesses in the range 1.5mm to 6.2mm. The refractive index of PC is 1.58 [39]. This value was used in the simulation for all PC materials.

The semi-crystalline thermoplastic examined was polyamide-6, otherwise known as PA6, or nylon-6. Samples filled with 20% long glass fibre were prepared by blending natural PA6 (Ultramid 8202HS, BASF company) [43] with 60% long glass-fibre PA6 (VLF 80211A, RTP company) [44]. Data for three thicknesses of this material were gathered using the line-scanning technique, and the transmission at each thickness recorded. For polyamide-6 with long glass fibre, a constant refractive index of 1.50 was used for all simulations [40].

5.2 Minima Search Algorithms

A method for finding parameters that would match experimental data both in transmission and the T-NPFD is needed. Several methods were employed. To match the T-NPFD, the experimental data was compared to the simulation-generated T-NPFD and the simulation variables were modified to minimize the objective difference, \( A_{rss} \), estimated using the same method as in Equation (37).

The first approach to this minima search was to use MATLAB’s function \texttt{fmincon} , which attempts to find the minimum of nonlinear functions with multiple variables. A script was written that called on the simulation to return a T-NPFD as a function of anisotropy, scattering and absorption. It then calculated the value of \( A_{rss} \) using the returned distribution and an experimentally determined T-NPFD. The index of refraction was set as a constant, along with the block parameters, the number of photons and resolution. These constant values are found in Table 4-2. Starting with an initial estimate, \texttt{fmincon} works within the script to find a minimum objective by altering the input variables and re-calculating the objective with the new simulation T-NPFD generated.

Using the \texttt{fmincon} function to approach this problem was ultimately unsuccessful. Attempts to minimize the objective were made using both the interior-point method and the trust-region method options within
Adjustments to the algorithm step size and initial guesses were also made. It was assumed that the problem has many local minima, a challenging problem for optimization algorithms. Moreover, matching the transmission was problematic with this approach. It is not clear how this algorithmic approach could be adjusted to include consideration of transmission data, which is wholly independent of the shape of the T-NPFD. To be considered a valid solution, a matched distribution must also accurately predict the transmission of laser power.

Instead, a so-called “brute force” approach was used. Rather than using \textit{fmincon} to minimize the objective, a second script was written that iteratively called on the simulation to return data on the distribution and the transmission for a given set of input parameters. As above, the index of refraction was set as a constant, along with the block parameters, the number of photons and resolution found in Table 4-2. For each iteration, the anisotropy, scattering and absorption coefficients were incremented successively, and the script calculated \( A_{rss} \) using the simulated T-NPFD and the experimental T-NPFD. The objective value \( A_{rss} \), the transmission and the three variables were written then to an Excel spreadsheet. Producing a complete set of simulations in this way typically required between one and five days of continuous processing, depending on the bounds chosen for each parameter and the increment size.

Within Excel, the program output was examined. Solutions that did not match the experimental transmission data to within \( \pm 5\% \) were discarded. To eliminate the remaining solutions, the procedure was repeated for the same material at a different thickness. The two groups of data were compared. Only sets of parameters that reproduced experimental T-NPFD and transmission results for both thicknesses were kept. Of the remaining sets of optical parameters, the group with the lowest value of \( A_{rss} \) was determined to be the ultimate solution. A small portion of the solutions data is presented in Appendix E for PA-6 and PC40GF. The script used to generate the solutions is listed in Appendix D.
Chapter 6. Using the Simulation to Reproduce Experimental Data

The brute force approach described in 5.2 was used to estimate the values of the Monte Carlo optical parameters for the materials in this study. As discussed in 5.1, two thermoplastic polymers were tested, a polycarbonate filled with four concentrations of glass fibre and a long-glass fibre reinforced polyamide-6. Brute force estimations of the optical parameters began with a coarse search. Broad parameter ranges were chosen, totaling 2,400 iterations. These could require between 48 and 72 hours on a Dell T3400 workstation. A coarse search was typically followed by a shorter, finer search in the region of potential solutions.

6.1 Polycarbonate

6.1.1 PC10GF

TEDD data PC10GF samples of thickness 2.3mm and 3.2mm of the 10%GF material were analyzed. Figure 6-1 and Figure 6-2 show the results of using the brute force approach to find the appropriate optical parameters for each sample thickness respectively. The T-NPFD of the unscattered laser beam is shown for reference.
Figure 6-1 T-NPFD for an in-focus Rofin laser scattered by a 2.3 mm PC10GF plate

Figure 6-1 shows the experimental TEDD data overlaid on a simulated T-NPFD for a 2.3 mm thick PC10GF sample. The model fits the experimental data well, with an $R^2=0.924$. A peak similar in height and width to the unscattered laser beam profile is observed. This indicates that at 2.3 mm, this material is not highly scattering.
Figure 6-2 T-NPFD for an in-focus Rofin laser scattered by a 3.2 mm PC10GF plate

Figure 6-2 shows the Monte Carlo simulation results for the same material and optical parameters but for a 3.2 mm thick sample. Again, the fit of the model to the experimental data is good, with an $R^2=0.910$. The peak value at this thickness is slightly lower than that at 2.3 mm, with a difference of 6% to the unscattered laser beam profile. This indicates higher laser dispersion as a result of increased scattering in a thicker part, as expected.

Although TEDD data was available only for 2.3 mm and 3.2 mm samples, transmission data was measured for additional thicknesses of PC10GF. With the same optical parameters used to generate the T-NPFDs shown in Figure 6-1 and Figure 6-2, new simulations were run to estimate the transmission at these thicknesses. These results are shown in Figure 6-3.
Agreement between the simulation and the experimental results is good and within experimental uncertainty. With only the 1.5, 2.3 and 3.2mm samples, the agreement appears better, suggesting that the estimate for the Monte Carlo optical parameters for this material could be improved. A T-NPFD taken at a third thickness could provide the data necessary to refine this estimate.

Using Chen’s modified Bouguer-Lambert Law [13] and the data presented in Figure 6-3, it is possible to calculate the apparent absorption coefficient. Equation (3) can be rewritten as:

\[ \ln(T_T) = \ln\left(\left(1 - R_T\right)\left(1 - \eta\right)\right) - A_1 D \]  \hspace{1cm} (39)

Figure 6-4 shows the relationship between \(\ln(T_T)\) and \(D\) for PC10GF.
From Figure 6-4, the graph is observed to have a slope of -0.0569. From Equation (39), the apparent absorption coefficient \( (A_i) \) for PC10GF is \( \approx 0.057 \, \text{mm}^{-1} \). From Table 6-1, the estimated absorption coefficient \( \mu_a \) is 0.05 mm\(^{-1} \). The difference between \( A_i \) and \( \mu_a \) is approximately 10%. The low level of scattering suggests that, for this type of material, Equation (39) provides a reasonable estimation of transmitted power for model simulation purposes.

**Table 6-1 Simulation solutions for PC10GF**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( g )</td>
<td>0.97</td>
<td>-</td>
</tr>
<tr>
<td>( \mu_a )</td>
<td>0.05</td>
<td>1/mm</td>
</tr>
<tr>
<td>( \mu_s )</td>
<td>0.6</td>
<td>1/mm</td>
</tr>
</tbody>
</table>

A comparison of the parameters presented in Section 6.1.5 will discuss these estimates as they related to glass fibre concentration.
6.1.2 PC15GF

The approach described in Section 57 was used to determine the optical parameters for 2.3mm and 3.2mm samples of PC15GF. Figure 6-5 and Figure 6-6 show the T-NPFD from the laser, model and experimental data for 2.3 mm and 3.2 mm thick plates respectively.

![Graph](image)

**Figure 6-5 T-NPFD for an in-focus Rofin laser scattered by a 2.3 mm PC15GF plate**

Figure 6-5 shows the simulated distribution fit to the experimental distribution well, with an $R^2=0.919$. As with PC10GF, the small difference between the scattered T-NPFD and the unscattered laser beam profile of 3% indicates that at this thickness, this material is not highly scattering.
Figure 6-6 T-NPFD for an in-focus Rofin laser scattered by a 3.2 mm PC15GF plate

Figure 6-6 shows the same results for a 3.2mm thick sample of PC15GF. Again, the simulation is in good agreement with experiment, with an $R^2=0.891$. As in the PC10GF, there is some indication of increased scattering in this thicker part, evidenced by a peak height 7% lower than the unscattered laser beam profile.

As with PC10GF, transmissions were measured and simulations performed for PC15GF samples at four thicknesses. The experiment and model transmission values are compared in Figure 6-7.
Figure 6-7 Transmission versus thickness for PC15GF plates, simulated and experimental

Agreement between the simulation and the experimental results is good. As with the PC10GF, the agreement is better using only the 1.5, 2.3 and 3.2mm samples. This indicates that this set of optical parameters may be further revised. Another set of experimental T-NPFD data at greater thickness could improve the estimate of the optical parameters.

As in Section 6.1.2, it is possible to calculate the apparent absorption coefficient $A_{1}$ from Figure 6-7. Figure 6-8 shows the relationship between $\ln(T_{T})$ and $D$ for PC15GF.
In Figure 6-8, the slope is -0.065. From Equation (39), the apparent absorption coefficient for PC15GF is \( \approx 0.065 \text{ mm}^{-1} \). From the estimated optical parameters shown in Table 6-2, \( \mu_a \) is 0.06. Similar to the results presented for PC10GF, the difference between \( A_I \) and \( \mu_a \) is again approximately 10%. Again, the low level of scattering suggests that for this type of material, Equation (39) provides a reasonable estimation of transmitted power for model simulation purposes.

Section 6.1.5 will present and discuss these parameters in the context of glass fibre concentration.
6.1.3 PC30GF

Results of fitting the simulation to TEDD data for PC30G, are shown in Figure 6-9 and Figure 6-10 for 2.6 mm and 3.2 mm thick plates.

![Graph showing T-NPFD for an in-focus Rofin laser scattered by a 2.6 mm PC30GF plate](image)

**Figure 6-9 T-NPFD for an in-focus Rofin laser scattered by a 2.6 mm PC30GF plate**

Figure 6-9 shows the experimental T-NPFD data overlaid on the simulated results for a 2.6mm thick, PC30GF. The simulation correlates well with experimental data, with an $R^2=0.913$. The difference in peak height of the scattered T-NPFD and the unscattered laser is 11% indicates PC30GF is not a highly scattering material. A lower peak compared to results in PC10GF and PC15GF due to the higher nominal thickness of this sample, as well as the increased scattering due to a higher glass fibre concentration, is expected.
Figure 6-10 T-NPFD for an in-focus Rofin laser scattered by a 3.2 mm PC30GF plate

T-NPFD results for the 3.2mm thick sample of PC30GF are shown in Figure 6-10. Again, the simulation is in good agreement with experimental data, with an $R^2=0.925$. The difference between the peak of the unscattered beam and the simulated T-NPFD is 16%, compared to a difference of 6% and 7% in PC10GF and PC15GF respectively for the same thickness. This indicates that PC30GF is a more scattering material.

Transmission data from measurements and simulations for 2.6mm and 3.2mm sample thicknesses are presented in Table 6-3 for PC30GF. Transmission at both thicknesses is in good agreement and within experimental uncertainty. Without more experimental measurements of transmission, little can be said regarding the quality of the fit.
Table 6-3 Transmission values for PC30GF at two thicknesses

<table>
<thead>
<tr>
<th>Thickness, mm</th>
<th>T-Experiment, %</th>
<th>T-Simulation, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.6</td>
<td>64.3</td>
<td>64.0</td>
</tr>
<tr>
<td>3.2</td>
<td>60.3</td>
<td>58.4</td>
</tr>
</tbody>
</table>

The Monte Carlo optical parameters used are presented below, in Table 6-4. A discussion of the parameters as they relate to glass fibre concentration is presented in Section 6.1.5.

Table 6-4 Simulation solutions for PC30GF

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>g</td>
<td>0.94</td>
<td>-</td>
</tr>
<tr>
<td>$\mu_a$</td>
<td>0.09</td>
<td>1/mm</td>
</tr>
<tr>
<td>$\mu_s$</td>
<td>0.9</td>
<td>1/mm</td>
</tr>
</tbody>
</table>

6.1.4 PC40GF

The final polycarbonate plate tested was PC40GF. Experimental and model T-NPFD results for a 2.2mm and a 3.1mm sample plate are Figure 6-11 and Figure 6-12.

![Figure 6-11 T-NPFD for an in-focus Rofin laser scattered by a 2.2 mm PC40GF plate](image)
The simulated T-NPFD for a 2.2 mm thick, PC40GF sample was fitted to experimental data, with an $R^2=0.965$. The difference between the T-NPFD peak and the unscattered laser is 7%, compared to a 2% difference in PC10GF at the same thickness indicates that this material is more highly scattering, as expected.

Simulation results for a PC40GF 3.1 mm thick plate fit experimental data with an $R^2=0.904$, indicating a good correlation. The difference between the peak of the T-NPFD at 2.2 mm and at 3.1 mm is 16%, as compared to a difference of 4% between the T-NPFDs at 2.3 mm and 3.2 mm for PC10GF. This indicates that PC40GF is a more scattering material than PC10GF.

Table 6-5 presents measured and simulated transmission data for the 2.2 mm and 3.1 mm PC40GF plates. As with PC30GF, more experimental measurements of transmission are necessary to comment on the quality of the fit.
Table 6-5 Transmission data for two thicknesses of PC40GF

<table>
<thead>
<tr>
<th>Thickness, mm</th>
<th>T-Experiment, %</th>
<th>T-Simulation, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.2</td>
<td>56.2</td>
<td>58.2</td>
</tr>
<tr>
<td>3.1</td>
<td>49.6</td>
<td>47.5</td>
</tr>
</tbody>
</table>

Table 6-6 presents the optical parameters estimated for PC40GF. Section 6.1.5 will present and discuss these parameters in the context of glass fibre concentration.

Table 6-6 Optical Parameters determined for PC40GF

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>g</td>
<td>0.94</td>
<td>-</td>
</tr>
<tr>
<td>( \mu_a )</td>
<td>0.14</td>
<td>1/mm</td>
</tr>
<tr>
<td>( \mu_s )</td>
<td>1.0</td>
<td>1/mm</td>
</tr>
</tbody>
</table>

6.1.5 Polycarbonate Results Summary
Polycarbonate at four different glass fibre concentrations was examined. For each material, two thicknesses were tested. The approach first described in 5.2 was used to estimate Monte Carlo optical parameters that would best reproduce the experimental T-NPFD and transmission data for the given thicknesses. The simulated beam profile distributions, for the 3.2 mm-thick samples are consolidated in Figure 6-13.
As the glass fibre content of PC increases, so does the light scattering, evidenced by a lower peak and wider tail. Figure 6-14 uses the parameters determined for the PC30GF to determine the beam profile distribution for several thicknesses. As with increased glass fibre concentration, increases in part thickness increase the degree of light scattering after it passes through the part, due to the longer path length to the weld interface.
Figure 6-14 Beam profile distributions for PC15GF at various thicknesses, zoomed for clarity.

Using the Monte Carlo optical parameters estimated for each sample of polycarbonate, the individual parameters are plotted as a function of glass fibre concentration in Figure 6-15. The figure shows that the absorption coefficient $\mu_a$ increases as glass fibre concentration increases. This is expected, as the introduction of glass fibre results in a greater number of scattering events, which in the simulation means more opportunities for a photon within the bulk volume to deposit a portion of its energy.

$\mu_s$, also appears to show an increase non-uniformly with glass fibre concentration. It shows no apparent increase across the 10%-15% concentration. As discussed in Section 2.1.1, Aden [10] estimated the optical properties of polycarbonate and reported a scattering coefficient of $\sim0.7$ mm$^{-1}$ for a 10% short glass fibre concentration and 0.8 mm$^{-1}$ for concentration of 15% short glass fibre. Differences between the model estimate and Aden’s result could be explained by difference in the polycarbonate used. This study reviewed samples provided by Osterman, while Aden had samples provided by Bayer Material Science.
Figure 6-15 Variation in optical parameters as glass fibre concentration increases; values in mm⁻¹ where applicable

The anisotropy factor $g$ decreases slightly with increases in glass fibre. As $g \to 0$, isotropic scattering increases and the photon has a greater probability to be scattered in any direction. As $g \to 1$, scattering becomes more forward directed, as discussed in Sections 3.1.5, 4.2 and 4.5.1. Therefore, it is expected that as more fibres are added to a material, overall scattering will tend to be more isotropic as, on average, light is more likely to be deviated from its original direction.

In addition to predicting exit beam profile distributions, the laser propagation model can also be used to examine the scattering pattern within the material. Figure 6-16 shows the relative absorption in a horizontal section of a 3mm and 6mm PC30GF part, respectively.
Figure 6-16 Laser light absorption within a 3mm (top) and 6mm PC30GF (bottom) part, XZ cross section

Figure 6-16 shows the relative strength of absorption in a cross section of PC30GF. The figures support the statement that 30%GF polycarbonate is not a highly scattering material. Although some scattering of light is visible in the 6mm simulation, the majority of the photons are not deviated significantly from the initial direction.
6.2 Polyamide-6

PA-6 with only one level of glass-fibre concentration (20%) was studied. Experimental T-NPFDs measured for a 1.5 mm, 2.2 mm and 3.1 mm thick plate are shown Figure 6-17, Figure 6-18 and Figure 6-19 respectively.

![Graph showing T-NPFD for a 1.5mm PA6 20% GF sample, experimental and simulated](image)

**Figure 6-17 T-NPFD for a 1.5mm PA6 20% GF sample, experimental and simulated**

Figure 6-17 shows the simulated T-NPFD for a 1.5mm thick plate fitted to experimental data. The fit is in good agreement with the experimental data, with an $R^2=0.876$. There is a change in peak-height of 13% between the simulated T-NPFD and the unscattered laser.
Figure 6-18 T-NPFD for a 2.2mm PA6 20% GF sample, experimental and simulated

Figure 6-18 shows the experimental and simulated T-NPFD for the 2.2mm thick plate with the unscattered laser beam profile for reference. The simulation is a good fit for the experimental data with an $R^2=0.966$. There is a change in peak height of 26% from the unscattered laser beam profile compared to a 7% change in PC40GF. This indicates that PA-6 is a significantly more scattering material. As PA-6 is a semi-crystalline polymer, this is thought to be due to the presence of crystallized portions of the polymer chain, which are likely to increase the scattering of transmitted light.
Figure 6-19 T-NPFD for a 3.1mm PA6 20% GF sample, experimental and simulated

Figure 6-19 shows the simulated T-NPFD for a 3.1 mm thick plate. As expected, the peak height is the lowest of the samples at 0.55 mm\(^{-1}\), representing a difference of 42% from the unscattered laser beam. This indicates the highest degree of scattering seen in any of the plates assessed. The simulated data fits the experimental data well, with an \(R^2=0.979\). Scattering at the tail ends more pronounced, compared to results for 2.2 mm and 1.5 mm plates. As discussed, photons in a thicker plate have a longer distance to travel to the weld interface. As a result, photons undergo more interactions, increasing the probability that they will be dispersed from their original location.

Transmission data for 1.5 mm, 2.2 mm and 3.1 mm thick plates was measured and simulated, and is presented in Figure 6-20. Agreement between the simulation and the experimental results is good. The decline in transmission with thickness increases supports the findings of Wang [19] discussed in Section 2.1.1.
The apparent absorption coefficient $A_1$ can be calculated from the data presented in Figure 6-20. Figure 6-21 shows the relationship between $\ln(T_T)$ and $D$ for PA6-LGF20%.
Using the slope in Figure 6-21 and Equation (39), the apparent absorption coefficient for this material is \( \approx 0.210 \text{ mm}^{-1} \), a typical value for glass fibre reinforce compounds [13]. From the optical parameters estimated (Table 6-7), \( \mu_a \) is 0.02 mm\(^{-1} \). This is lower than the absorption coefficient observed in PC and lower than the apparent absorption coefficient \( A_t \) calculated from Figure 6-21. One explanation might be that spherulites in real semi-crystalline polymers are more likely to scatter than absorb energy, due to the change of index of refraction that across the amorphous-crystalline boundary. Thus, the high total amount of absorption that takes place in PA-6 results from a high average number of steps.

As expected, the scattering coefficient \( \mu_s \) is higher than those observed for PC.
### Table 6-7 Simulation solutions for PA6-LGF20%

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>g</td>
<td>0.94</td>
<td>-</td>
</tr>
<tr>
<td>( \mu_a )</td>
<td>0.02</td>
<td>1/mm</td>
</tr>
<tr>
<td>( \mu_s )</td>
<td>3.0</td>
<td>1/mm</td>
</tr>
</tbody>
</table>

#### 6.2.1 Polyamide-6 Results Summary

PA-6 reinforced with 20% concentration glass fibre was examined. Three thicknesses were tested. Compared to the results of the analysis of polycarbonate, PA6 is a far more scattering material, likely due to its semi-crystalline nature, as discussed in Section 6.2. The difference in scattering between PC and PA-6 is evidenced primarily by the value of \( \mu_s \). In PA-6, the value of this coefficient is three times larger than PC40GF, the PC sample with the highest scattering coefficient.

The simulated T-NPFDs for the three thicknesses assessed are shown in Figure 6-22.
PA6 is a highly scattering material. As the thickness increases, so does the light scattering.

The absorption within the part can also be observed. Figure 6-23 shows sections of PA6 reinforced with 20% GD at 3mm and 6mm thicknesses. In contrast to polycarbonate, scattering is immediately apparent at 3mm. At 3mm the beam distribution absorbed near the interface is visibly dispersed. At 6mm, light absorbed near the interface is distributed across a much wider range, compared to the same thickness in PC30GF (Figure 6-16), as expected.
Figure 6-23 Laser light absorption within a 3mm and 6mm in PA-6 20% GF, XZ cross section

The absorption shown in Figure 6-23 indicates that energy is absorbed over a 10 mm range. This suggests that Beer’s Law is not appropriate for this material, as scattering is significant.
Chapter 7. Conclusion

A program based on the Monte Carlo method for photon transport was written to simulate light propagation through a polymer in laser transmission welding.

The technique simulates photon paths through the material according to the input laser beam profile in order to predict the beam profile distribution as a result of scattering through reinforced or otherwise scattering polymers. The simulation is highly adaptable and can be configured to apply a wide range of incoming beam profiles, part geometries and materials. A method for obtaining the appropriate optical parameters for a given material is also discussed, and the results of applying this method to glass-reinforced polycarbonate and polyamide samples are presented. Fits are generally in good agreement (R>0.90) and the simulation accurately predicted transmissions to within 5% of the experimentally determined values. The simulations also allowed the prediction of transmission and power distributions at other thicknesses.

7.1 Recommendations

- The program uses an incoming beam profile distribution to scale same the photon paths repeatedly and adds them to a master matrix, to save the large computation times associated with running thousands of photons repeatedly (3.2). Modification of the program to instead utilize each discrete position on the incoming beam profile distribution as a starting point for a weighted number of photons could better simulate scattering effects, particularly when the beam is close to part edges, for example.

- The Henyey-Greenstein function is used as the phase function to determine the deflection angle (3.1.5) for scattered photons. While straightforward and analytically simple, the HG function does not accurately reproduce the backscatter peaks seen in highly scattering material, potentially leading to inaccurate predictions of reflectance and transmittance. A modification to the phase function is suggested should the simulation fail to accurately describe reflectance, which was not
examined in this thesis. The “modified Henyey-Greenstein”, at the cost of additional optical parameters, or adaptation of a true Mie phase function are both candidates.

- The simulation consists of a series of MATLAB functions which must be called from the command window. Development of a graphical user interface for the simulation, and packaging into a file executable without MATLAB would improve the program’s usability.
Bibliography


Appendix A

The MATLAB code for the laser propagation model is listed here. The function “laserprop” accepts the four Monte Carlo optical parameter. The input beam profile must first be generated by the script LM_BPD_Proc_2013mar13gzap.m, listed in Appendix B.

```matlab
function [MZhigh] = laserprop(g,mua,mus,nmat)
%This function returns the beam profile at the weld interface based on the
%four Monte-Carlo optical parameters propagation. It includes code that can
%uncommented for the analysis of TEDD/line-scanning data. Written by
Alexander Parkinson through 2012-2013

close all

% tic
resscale = 2;
%Resolution and number of photons to be simulated. These are the primary
%determinants of how long this program will take to run.

X = 10;
Y = 10;
Z = 3.2;
laserd = 2;
%Physical size of our "block", in mm, and the diameter of the laser.

Nx = 5*X*resscale;
Ny = 5*Y*resscale;
Nz = 5*Z*resscale;
%Number of bins - "resolution". Modifying the resscale variable changes the
%resolution - I find that numbers between 1 and 10 are sufficient (more
%simply requires too much memory at this point (2012). Nx,Ny and Nz should
%ultimately be a multiple of 5. Using resscale = 2 or 3 is a great place to
%start.

dx = X/Nx;
dy = Y/Ny;
dz = Z/Nz;
res = laserd/dx;
%The volume of each bin is given by dx*dy*dz.

[~,~,~,~,~,~; Zhigh] =
laserpropprofile(g,Nphotons,mua,mus,Nx,Ny,Nz,dx,dy,dz,X,Y,Z);
%Calls on laser prop profile to return the distribution of photons at the
%weld interface from a single point source of photons located above, in the
%middle of the part. At this point, we're only really interested in Zhigh,
%the distribution at the interface. To enable the others, you'll need to go
%into the laserpropprofile and un-comment the calculations of the other
%matrices.

M = zeros(Nx+res,Ny+res,Nz);
MZhigh = zeros(Nx+res,Ny+res);
S = zeros(res,res);
```
These define the "master" matrix $M$ - a larger matrix into which $Q$ is placed and collected, and the "scaling" matrix $S$, the matrix that contains the relative strength of the laser in corresponding X-Y locations - scales the $Q$ summation into the $M$ matrix for that locale. Similarly, $M_{\text{high}}$ is the final collection of photons at the interface, added up according to the weights assigned by the input beam.

```matlab
xPSmallNorm = dlmread('xPSmallNorm1.txt');
yPSmallNorm = dlmread('yPSmallNorm1.txt');
NPFDxy = dlmread('NPFDxy1.txt');
% Pulls the relevant beam profile information from the text files located in the same folder as this program.
yRangeTemp = zeros(res,1);
xRangeTemp = zeros(res,1);
x = -laserd/2;
for i=1:res
    y = -laserd/2;
    for j=1:res
        S(i,j) = griddata(xPSmallNorm,yPSmallNorm,NPFDxy,x,y);
        if isnan(S(i,j)) == 1
            S(i,j) = 0;
        end
        yRangeTemp(j) = y;
        y = y+dy;
    end
    xRangeTemp(i) = x;
    x = x+dx;
end
% For
% Interpolates the beam to match the resolution of the Monte Carlo portion. In other words, it constructs the scaling matrix

for i=1:res
    for j=1:res
        ti = i;
        for a=1:Nx
            tj = j;
            for b=1:Ny
                MZhigh(ti,tj) = Zhigh(a,b)*S(i,j)+MZhigh(ti,tj);
            end
            tj = tj+1;
        end
        ti = ti+1;
    end
end
% For
% This loop scales the $Z_{\text{high}}$ output. Note that in the thesis, $Z_{\text{high}}$ is referred to as the $Z$-face matrix, $FZ$, while $Z_{\text{low}}$ is called $FZ0$.

% outputBeamProfileX(:,2) = sum(MZhigh,1);
% outputBeamProfileY(:,2) = sum(MZhigh,2);
% for i=2:Nx+res
%     outputBeamProfileX(i,1) = outputBeamProfileX(i-1,1)+dx;
% end
% for i=2:Ny+res
%     outputBeamProfileY(i,1) = outputBeamProfileY(i-1,1)+dx;
% end
```
% outputBeamProfileX = normalise(outputBeamProfileX);
% outputBeamProfileY = normalise(outputBeamProfileY);
% defines and conditions output beam profiles
% PoPkX = dlmread('PoPkX.txt');
% PoPkY = dlmread('PoPkY.txt');
% TEDDChenVarsX = dlmread('TEDDChenVarsX.txt');
% TEDDChenVarsY = dlmread('TEDDChenVarsY.txt');
% outputBeamProfileX(:,1) = outputBeamProfileX(:,1) - (laserd+X)/2 + shiftX;
% outputBeamProfileY(:,1) = outputBeamProfileY(:,1) - (laserd+Y)/2 + shiftY;
% TEDDChenX = dlmread('TEDDChenEstimateX.txt');
% TEDDChenY = dlmread('TEDDChenEstimateY.txt');
% xRangeX = TEDDChenX(:,1);
% xRangeY = TEDDChenY(:,1);
% aX = interp1(outputBeamProfileX(:,1),outputBeamProfileX(:,2),xRangeX);
% aY = interp1(outputBeamProfileY(:,1),outputBeamProfileY(:,2),xRangeY);
% objX = sum((aX - TEDDChenX(:,2)).^2);
% objY = sum((aY - TEDDChenY(:,2)).^2);
% % This section is for using laserprop to compare TEDD data. If you have
% % some TEDD data, then you can uncomment and use this section.

end
%Masterfunction

function [Q,Xlow,Xhigh,Ylow,Yhigh,Zlow,Zhigh] =
laserpropprofile(g,Nphotons,mua,mus,nmat,Nx,Ny,Nz,dx,dy,dz,X,Y,Z)
%This function fires photons into the part for the given parameters, and
%returns the collections of photons at all the part faces as matrices.
global transmission

nair = 1;
mut = mua+mus;
dirthresh = 0.99;
%Dirthresh is a threshold that determines when the rules change for photon
%scattering - how aligned with the Z axis the photon must be before the
%rules change
chance = 0.1;
weightthresh = 0.0001;
%What is the chance that a photon die after the threshold is crossed, and
%what is the threshold?

Xlow = zeros(Ny,Nz);
Xhigh = Xlow;
Ylow = zeros(Nx,Nz);
Yhigh = Ylow;
Zlow = zeros(Nx,Ny);
Zhigh = Zlow;
Q = zeros(Nx,Ny,Nz);
%xycount = zeros(Nphotons,2);

%These are our catchment matrices - they'll record the photon weights that
%escape from these surfaces. For example, if a photon escapes from the X=0
%(i.e. "Xlow" surface), the weight that escapes is recorded in a bin at the
%Y-Z coordinates of the event. Q is the catchment matrix that collects
%energy deposited from scattering events in the plastic, away from %boundaries.

%Now we begin with the launch of a photon. This is the part of the program %I've had difficulty getting compartmentalised, because I have bad %programming habits and so often want to resort to a GO-TO function.

for counter=1:Nphotons

x = X/2;
y = Y/2;
z = 0;

%These are the start coords for a photon. It stands to reason then that the %z=0 is the top surface of the transparent plastic part. We will assume the %top surface of the black plastic part is z=Z (defined). Thus, every photon %begins at the dead center of the part. We can discuss techniques for %simulating gaussian/tophat/etc beams, of course, by manipulating the %starting location and changing the number of photons launched from that %point
ux = 0;
uy = 0;
uz = 1;

%This is the start velocity vector for the photon (remember |u| = 1 always) %- headed vertically into the plastic. We will assume it starts infinitely %close to, but under the surface of the transparent plastic - so every %photon considered is transported through the plastic - i.e., there's no %chance the photons can be reflected as they begin

timetoend = 2;
%This variable is changed when a photon dies, so the while loop quits
w = 1;
%The photon has a "weight" of 1
while (timetoend == 2)

%Now we discuss step size. Each step size is dependent on the extinction %coefficient, mut

step= -log(rand(1))/mut;
%That's the natural logarithm, and this will randomise each step-size. %Remember mut = mua + mus, so the larger the scattering or absorption %coefficient, the smaller the step size. Units are important!
x = x + ux*step;
y = y + uy*step;
z = z + uz*step;
%The location of the photon is updated according to the step size.

%These are the photon boundary event rules:
while (z > 2) || (x > X) || (y > Y) || (z < 0) || (x < 0) || (y < 0)
[x,y,z,ux,Xhigh,Xlow,w] = 
checkbound(x,y,z,ux,uy,uz,dy,dz,X,Xhigh,Xlow,w,step,nmat,nair);
[y,z,x,uy,Yhigh,Ylow,w] = 
checkbound(y,z,x,ux,uy,uz,dx,dz,Y,Yhigh,Ylow,w,step,nmat,nair);
[z,x,y,uz,Zhigh,Zlow,w] = 
checkbound(z,x,y,uz,ux,uy,dx,dy,2,Zhigh,Zlow,w,step,nmat,nair);
end
Okay. The photon now has a new position, and has either been reflected, or none of our IF statements have been triggered because it is still far away from the boundaries. We must now scatter a little of the photon's weight - update this into energy deposited in our Q matrix.

\[ i = \text{fix}(x/dx)+1; \]
\[ j = \text{fix}(y/dy)+1; \]
\[ k = \text{fix}(z/dz)+1; \]

Like in the preceding border check statements, this rounds our photon into the nearest bin. Because the fix function rounds towards zero, a photon always deposits its energy in the next bin. This is to avoid the program attempting to access a matrix/vector index of 0.

\[ Q(i,j,k) = Q(i,j,k) + w*mua/mut; \]

Q matrix is updated with the weight of the photon lost as its energy is deposited in a scattering event (remember a scattering event occurs with every step).

\[ w = w*mu_s/mu_t; \]

Weight of the photon is updated accordingly.

```
if (w < weightresh)
    if (rand(1) <= chance)
        w = w/chance;
    else
        timetoend = 1;
end
```

%%%%%%

Now we have to find a new direction for the photon to propagate along. The Henyey-Greenstein function provides the description.

\[ c_1 = (1+g^2-((1-g^2)/(1-g+2g*rand(1)))^2)/(2*g); \]
\[ s_1 = \sqrt{(1-c_1^2)}; \]
\[ \phi = \pi*rand(1); \]
\[ c_2 = \cos(\phi); \]
\[ s_2 = \sin(\phi); \]
\[ \psi = \sqrt{(1-u_z^2)}; \]

```
if (abs(u_z) > dirthresh)
    if the uz component is very large - i.e. the photonic direction is almost parallel with the z axis, the rules change. This is the application of the dirthresh variable. I'm not sure what should govern our choice of the value of this variable.
    u_{xx} = s_1*c_2;
    u_{yy} = s_1*s_2;
    if (u_z >= 0)
        u_{zz} = c_1;
    else
        u_{zz} = -c_1;
else
    u_{xx} = s_1*(ux*u_z*c_2-uy*s_2)/psi+ux*c_1;
    u_{yy} = s_1*(uy*u_z*c_2+ux*s_2)/psi+uy*c_1;
    u_{zz} = -s_1*c_2*psi+u_z*c_1;
end
```
unitytest = uxx^2 + uyy^2 + uzz^2;
    if (unitytest > 1.00001) || (unitytest < 0.99995)
        disp('Direction cosines dont sum to one')
    end
%Rules surrounding the photon's new trajectory
ux = uxx;
uy = uyy;
uz = uzz;
%Photon direction is updated.

% sumZlow = sum(sum(Zlow));
sumZhigh = sum(sum(Zhigh));
% sumXlow = sum(sum(Xlow));
% sumXhigh = sum(sum(Xhigh));
% sumQ = sum(sum(sum(Q)));
transmission = sumZhigh/Nphotons;
end
end
end

%This is the checkbound function, that checks whether the photons have hit
%the boundary and repels them accordingly
function [var1, var2, var3, dir1, MatrixHigh, MatrixLow, w] = ...
    checkbound(var1, var2, var3, dir1, dir2, dir3, res2, res3,...
        size1, MatrixHigh, MatrixLow, w, step, nmat, nair)
    if (var1 < 0) || (var1 > size1)
        %If this is happening, then the photon is trying to escape the material -
        %call the guards.
        tempvar = var1;
        %This is a temporary variable that allows us to remember whether the
        %photon is attempting to escape the top of bottom
        var1 = var1 - dir1*step;
        var2 = var2 - dir2*step;
        var3 = var3 - dir3*step;
        %The photon's step is retraced to its last position.
        if (tempvar > var1)
            stepshort = abs((size1-var1)/dir1);
        else
            stepshort = abs(var1/dir1);
        end
        %New step size is calculated to help the photon get exactly to the border
        var1 = var1 + dir1*stepshort;
        var2 = var2 + dir2*stepshort;
        var3 = var3 + dir3*stepshort;
        %The photon takes the new step and is exactly at the border
\[ c_1 = \text{dir1}; \]
\[ s_1 = \sqrt{1-c_1^2}; \]
\% Cosine of the incident velocity, and the corresponding sine
\[ s_2 = s_1 \times n_{\text{mat}}/n_{\text{air}}; \]
\textbf{if} (\text{\textit{s2} > 1})
\[ \text{dir1} = -\text{dir1}; \]
\textbf{else}
\[ c_2 = \sqrt{1-s_2^2}; \]
\% Sine of the transmitted velocity, and the corresponding cosine

\% Now we use the Fresnel reflection equation to calculate the internal
\% reflectance - how "much" of the photon will be reflected
\[ \text{\textit{critical}} = \text{asin}(n_{\text{air}}/n_{\text{mat}}); \]
\% Critical angle
\textbf{if} (\text{\textit{asin(s1)}} \text{\textit{\geq critical}})
\[ \text{Rs} = 1; \]
\[ \text{Rp} = 1; \]
\textbf{else}
\[ \text{Rs} = \text{abs}((n_{\text{mat}}\times\text{abs(c1)}-n_{\text{air}}\times\text{abs(c2)})/(n_{\text{mat}}\times\text{abs(c1)}+n_{\text{air}}\times\text{abs(c2)}))^2; \]
\[ \text{Rp} = \text{abs}((n_{\text{mat}}\times\text{abs(c2)}-n_{\text{air}}\times\text{abs(c1)})/(n_{\text{mat}}\times\text{abs(c2)}+n_{\text{air}}\times\text{abs(c1)}))^2; \]
\textbf{end}
\[ \text{R} = (\text{Rs}+\text{Rp})/2; \]
\% Fresnel equations to calculate the internal reflection coefficient

\% Now we need to locate the var2-var3 coordinates of the escape in integers, so
\% we can update the \textit{varlow/high} matrix
\[ i = \text{\textit{fix}}(\text{\textit{var2}}/\text{\textit{res2}})+1; \]
\[ j = \text{\textit{fix}}(\text{\textit{var3}}/\text{\textit{res3}})+1; \]
\% Rounds down - so if the photon is located at \textit{var1} = 14.34 after step, it is % put in bin 15. This isn't extremely accurate, but it avoids the matrix 0 % problem
\[ [a,b] = \text{size}(\text{MatrixLow}); \]
\[ [c,d] = \text{size}(\text{MatrixHigh}); \]
\textbf{if} (\text{\textit{tempvar} < 0})
\[ \textbf{if} (i < a) \&\& (j < b) \&\& (i > 0) \&\& (j > 0)
\[ \text{MatrixLow}(i,j) = \text{MatrixLow}(i,j) + (1-R)\times w; \]
\% \textit{Zlow} - the surface at the event - matrix is updated\n\textbf{end}
\textbf{end}

\textbf{if} (\text{\textit{tempvar} > \textit{size1}})
\[ \textbf{if} (i < c) \&\& (j < d) \&\& (i > 0) \&\& (j > 0)
\[ \text{MatrixHigh}(i,j) = \text{MatrixHigh}(i,j) + (1-R)\times w; \]
\% \textit{Zhigh} - the surface at the event - matrix is updated\n\textbf{end}
\textbf{end}
\% These statements address a slight problem I suspect is related to the reflection;
\% they are crutches to prevent attempting to access out-of-bounds matrix elements
\[ w = R\times w; \]
\[ \text{dir1} = -\text{dir1}; \]
\% Photon's weight is updated, and its velocity updated for a reflection\n\textbf{end}
\texttt{var1 = var1+(step-stepshort)*dir1;}
\texttt{var2 = var2+(step-stepshort)*dir2;}
\texttt{var3 = var3+(step-stepshort)*dir3;}
\texttt{\%
\texttt{The photon continues along its original step but now with a new}
\texttt{\%trajectory}
end}
Appendix B

The script for formatting pinhole beam data, LM_BPD_Proc_2013mar13gzap.m is presented here. This script was originally written by Gene Zak, PhD. and edited for use with laserprop.m.

```matlab
% File for processing the beam profiling data
% Assumes the "BP_Dat" data file has the following columns:
% Time (ms)  Xpos (counts)  Ypos (counts) Meter_Output (Volts)
% Created by G. Zak 24-Aug-2005
% modified by G. Zak 21-mar-2006:
% (1) automating import of data from the text "grepped" files
% (2) controlling the plots & displaying the filename on the plots
% (3) resizing the beam profile data array to be more compact for input
% into the program producing the Heat Generation input for ANSYS
% Modified by A. Parkinson 13-Feb-2013
% (1) Prints results formatted for use in laserprop.m

disp('Beam Profile program started')
% if file name entry is skipped, assume the BP_Dat is already in Matlab workspace
yy=input('Enter file name? (y/n)', 's');
%yy='n';
if yy=='y'
    % interactively asks for the file name of the input data "*.txt" file
    [filename, pathname] = uigetfile('*.txt', 'Find Beam Profile Data input file');
    if isequal(filename,0)|isequal(pathname,0)
        disp('EXITING PROGRAM: File not found')
        return
    else
        disp(['File located in ', pathname])
        disp(['File ', filename, ' read in'])
    end
    BPDtmp = dlmread(fullfile(pathname, filename), ' ');  
    BP_Dat = BPDtmp(:,[1 2 4 7]);  % select 1st, 2nd, 4th, and 7th columns from the imported data
end %if

% Assume that at this point the Beam Profile data is stored in a variable "BP_Dat"

% Convert Volts to meter mW using relationship:
% Power (mW) = (measuredVolts - meterOffsetVolts)*mWperV
% typical conversion factors are 3000 or 1000, depending on the meter range
% used to collect the data
conFactAns = input('Enter conversion factor of mW per V (rtn=3000):');
if isempty(conFactAns),
    mWperV = 3000/2;
else,
    mWperV = conFactAns/2;
end
```
meterOffsetVolts = 0.0356; %0.057;
power_mW = (BP_Dat(:,4) - meterOffsetVolts)*mWperV;

% Convert time to sec & counts to position in mm (1600 counts = 1 mm)
% Create a new matrix with converted values
BPD = [BP_Dat(:,1)/1000 BP_Dat(:,2)/1600 BP_Dat(:,3)/1600 power_mW];

% Position increments in X and Y are assumed to be (in mm)
incrX = 0.1; incrY = 0.1;

% Calculate number of positions measured along X and Y
nX = round(1+(max(BPD(:,2))-min(BPD(:,2)))/incrX);
nY = round(1+(max(BPD(:,3))-min(BPD(:,3)))/incrY);

% for most cases nX=30 and nY=30; however other numbers were used as well
disp(['Number of position increments along X = ' num2str(nX) ' and along Y = ' num2str(nY) ']);

% Get total number of measurements
nMeas = length(BP_Dat(:,1));

% Define number of repeated measurements at each sample point
nRep = 10;
nSamples = nMeas/nRep;

% empty array which will contain averaged data with three columns: X Y Power
BPD_ave = zeros(nSamples, 3);
% Calculate averaged values & place in a new matrix
for iSample = 1:nSamples,
    dataStart = (iSample-1)*nRep+1; % Sequence: 1, 11, 21, ... for nRep=10
    BPD_ave(iSample,1:2) = BPD(dataStart:2:3); % transfer X & Y coordinates to averaged array
    BPD_ave(iSample,3) = mean(BPD(dataStart:dataStart+nRep-1,4)); % calculate average of nRep meas-ts
end

% Manipulate the BPD_ave array to arrange it so that the measured powers
% are in a 2-D array with each measurement located at X(J), Y(I) of the
% array, where I & J are array row & column indexes. Thus, for example,
% location (I,J) = (1,2) corresponds to the first row, second column. This
% would correspond to the second position measured along X and first
% position along Y.
powerXY = reshape(BPD_ave(:,3),nY,nX);

% rearrange the above matrix as specified above
powerXY = flipud(powerXY); % reorders the Y distances to be in increasing sequence
peakPowerXY = max(max(powerXY));

% Estimate of total power in the beam (Watts)
totPowerEst = (sum(sum(powerXY)))*(incrX*incrY)/(3.1415*(0.2^2)/4))/1000;
disp(['Total power estimate = ' num2str(totPowerEst) ' Watts']);

% find positions measured along X & Y
Temp = reshape(BPD_ave(:,1),nY,nX);
xPos = Temp(1,:);
ypos = BPD_ave(nY:-1:1,2);

xPosNorm = xPos - mean(xPos);
yPosNorm = yPos - mean(yPos);
% Select if & how the beam profile data array will be limited in X and Y
limAnswer=input('Beam profile limit type select: 1-none, 2-manual, 3-auto (rtn=3)');
if isempty(limAnswer),
    limAnswer=3; % default setting - if return is pressed
elseif limAnswer>3 | limAnswer<1,
    error('Choose number from 1 to 3')
end

% no limits on the original beam profile data array
if limAnswer==1,
    xPSmall = xPos;
    yPSmall = yPos;
    powerXYSmall = powerXY;
else,
    % manual limits on the original beam profile data array
    if limAnswer==2,
        xPLim = input('Enter lower & upper beam limits for X [lower upper] :');
        yPLim = input('Enter lower & upper beam limits for Y [lower upper] :');
        xPIndx = xPosNorm>=xPLim(1) & xPosNorm<=xPLim(2);
        yPIndx = yPosNorm>=yPLim(1) & yPosNorm<=yPLim(2);
    end %if limAnswer==2
    % Automatic setting of upper and lower limits
    % by finding which elements of the array are above some low-level threshold
    if limAnswer==3,
        threshVal = input('Enter threshold value in percent:');
        threshVal = threshVal/100;
        % Find where in the original data array the power values are above
        % set threshold
        threshPowerXYIndx = powerXY>=threshVal*peakPowerXY;
        % find first and last occurrences of non-zero values along each axis
        sumXindx = sum(threshPowerXYIndx,1);
        sumYindx = sum(threshPowerXYIndx,2);
        tempX = find(sumXindx>0);
        tempY = find(sumYindx>0);
        xLindx = tempX(1); xHindx = tempX(end);
        yLindx = tempY(1); yHindx = tempY(end);
        xPIndx = xLindx:xHindx;
        yPIndx = yLindx:yHindx;
    end %if limAnswer==3
    xPSmall = xPosNorm(xPIndx);
    yPSmall = yPosNorm(yPIndx);
    powerXYSmall = powerXY(yPIndx,xPIndx);
end %if limAnswer==1

% Calculate shift of X and Y coordinates to centre beam within the Data % array

103
% Select how the beam profile data array will be shifted in X and Y
shiftAnswer=input('Beam profile shift select: 1-midpoint of X & Y, 2-weighted centre (rtn=1)');
if isempty(shiftAnswer),
    shiftAnswer=1; % default setting - if return is pressed
elseif shiftAnswer>2 | shiftAnswer<1,
    error('Choose number from 1 to 2')
end

if shiftAnswer==1,
    % shift coordinates to midpoint of the X and Y ranges
    xShift = mean(xPSmall);
    yShift = mean(yPSmall);
end
if shiftAnswer==2,
    % shift coordinates to weighted centre of the beam distribution
    xShift = round(sum(powerXYSmall*xPSmall)/sum(sum(powerXYSmall))*20)/20;
    % round off to nearest 0.05 mm
    yShift = round(sum(yPSmall*powerXYSmall)/sum(sum(powerXYSmall))*20)/20;
    % round off to nearest 0.05 mm
end
xPSmallNorm = xPSmall - xShift;
yPSmallNorm = yPSmall - yShift;

xyAxisLim = max(max(abs(xPSmallNorm)), max(abs(yPSmallNorm)));
xAreaSize = xPSmallNorm(end)-xPSmallNorm(1);
yAreaSize = yPSmallNorm(end)-yPSmallNorm(1);

disp(['Beam profile array area size is X = ' num2str(xAreaSize,4) ' mm and Y = ' num2str(yAreaSize,4) ' mm'])

disp(['Beam profile array size is ' num2str(size(powerXYSmall))])

% Normalizing the powerXY to obtain Normalized Power Flux Distribution (NPFD):
% power measurements at each point are normalized so that the sum of all normalized values multiplied by the increment in X and Y is equal to one
NPFDxy = powerXYSmall / (sum(sum(powerXYSmall)) * incrX * incrY);

% define which of the following plots will be plotted
% put 1 to plot & 0 not to plot; for example [1 1 0 0] activates 1st & 2nd plots and turns off 3rd & 4th
PLT_ON = [1 1 0 0];

%% PLOT: 3-D SURFACE %%%%%%
% Use surf(X,Y,Z) function to plot a 3-D surface profile of the data
if PLT_ON(1),
    figure();
    surf(xPosNorm, yPosNorm, powerXY_Norm);
    surf(xPSmallNorm, yPSmallNorm, NPFDxy);
    xlabel('X (mm)'); ylabel('Y (mm)'); zlabel('NPFD 1/mm^2');
    set(gca,'ZLim', [0 1]);
    xlim([-1 1]*xyAxisLim);ylim([-1 1]*xyAxisLim)
    colorbar('vert');
    hT = title(['File: ' filename]);
    set(hT,'Interpreter','none'); % disables Tex interpreter -- does not create super/subscripts
end
%%%%%% PLOT: CONTOURS %%%%%%%
if PLT_ON(2),
    figure(2);
    peakNPFDxy=max(max(NPFDxy));
    contourBounds = [.135:(0.95-0.135)/4:0.95];
    contourf(xPSmallNorm, yPSmallNorm, NPFDxy, contourBounds*peakNPFDxy);
end % "contour" is an alternative command gives line contours instead of solid colours

%    contourf(xPosNorm, yPosNorm, powerXY_Norm, contourBounds*peakNPFDxy); %
% "contour" is an alternative command gives line contours instead of solid colours

xlabel('X (mm)');
ylabel('Y (mm)')

% xlim([-1 1]*xyAxisLim); ylim([-1 1]*xyAxisLim)
axis equal
legend(num2str(contourBounds', 3))
hT = title(['File: ' filename]);
set(hT, 'Interpreter', 'none');
end

% Estimate sums along X and Y for comparison with knife-edge-based data
sumX = sum(NPFDxy,1)*incrX;
sumY = sum(NPFDxy,2)*incrY;

%%%%%% PLOT: Y NPFD %%%%%%%
if PLT_ON(3),
    figure;
    plot(yPSmallNorm, sumY)
    xlabel('Y (mm)'); ylabel('NPFD (1/mm)');
    hT = title(['File: ' filename]);
    set(hT, 'Interpreter', 'none');
end

if PLT_ON(4),
    figure;
    plot(xPSmallNorm, sumX)
    xlabel('X (mm)'); ylabel('NPFD (1/mm)');
    hT = title(['File: ' filename]);
    set(hT, 'Interpreter', 'none');
end

disp('Beam Profile program finished')
fileID = fopen('xPSmallNorm1.txt', 'w');
fprintf(fileID, '%12.8f\n', xPSmallNorm);
fclose(fileID);
fileID = fopen('yPSmallNorm1.txt', 'w');
fprintf(fileID, '%12.8f\n', yPSmallNorm);
fclose(fileID);
dlmwrite('NPFDxy1.txt', NPFDxy, '');
Appendix C

This script uses the analytical model developed by Chen et al. [12] to normalize raw TEDD data for use in laserprop.m. It also estimates the parameters $\sigma$, $\delta$ and $\Psi'(0)$ used in Equation (8). Finally, it can plot a profile of the estimated T-NPFD, according the analytical model.

%This script will estimate the value of delta,sigma and psiStar. The %arguments are your initial guesses
%Written by Alexander Parkinson, February 2013.
clear all
close all
disp('Welcome to the TEDD-Chen Variable Estimator!')
disp('Please hit enter to find your unscattered X-Dir beam profile data
(Psi(x)): ')
pause;
[filename, pathname] = uigetfile('*.txt','Find your X-Dir Psi(x) Data input
file: ');
Psi = dlmread([pathname filename]);
disp('File read. Please hit enter to find your X-Dir Po/Pk data file - this
is required: ');
pause;
[filename,pathname] = uigetfile('*.txt','Find your X-Dir Po/Pk Data input
file: ');
PoPk = dlmread([pathname filename]);
dlmwrite('PsiX.txt',Psi);
dlmwrite('PoPkX.txt',PoPk);

% disp('Next, we need some estimates from you. Please give as your initial
estimate of ')
% x0(1) = input(' Delta: ');
% x0(2) = input(' Sigma: ');
% x0(3) = input(' PsiStar: ');
% disp('One more set of estimates needed! Enter them as requested: ')
% lb(1) = input(' Lower Bound, Delta: ');
% ub(1) = input(' Upper Bound, Delta: ');
% lb(2) = input(' Lower Bound, Sigma: ');
% ub(2) = input(' Upper Bound, Sigma: ');
% lb(3) = input(' Lower Bound, psiStar: ');
% ub(3) = input(' Upper Bound, psiStar: ');
% disp('Thank you! Finally ready to get started. Hit enter to compute!')
% pause;
lb = [0.01 0.01 0.01];
ub = [1 6 1];
x0 = [0.2 0.2 0.2];
options = optimset('Display','iter','MaxIter',10000,'Algorithm','interior-
point','MaxFunEvals',10000);
[x,fval] = fmincon(@TEDDChenObjCreatorX,x0,[],[],[],lb,ub,[],options);
dlmwrite('TEDDChenVarsX.txt',x);

delta = x(1)
sigma = x(2)
psiStar = x(3)
\[
\tau = \frac{1}{\psiStar}
\]

\[
\text{[npfd, xRange]} = \text{brute20130326}(\text{delta, sigma, psiStar, } [3:0.1:3, 'X']);
\]

\[
\text{TEDDChenEstimateX} = \text{[xRange npfd]};
\]

\[
\text{dlmwrite('TEDDChenEstimateX.txt', TEDDChenEstimateX)};
\]

\[
\text{function [obj] = TEDDChenObjCreatorX(x0)}
\]

\[
\%This function returns the objective values for estimating values of sigma \%
\%delta and psiStar.
\]

\[
\text{Psi} = \text{dlmread('PsiX.txt')};
\]

\[
\text{PoPk} = \text{dlmread('PoPkX.txt')};
\]

\[
\text{xRange} = \text{PoPk}(:,1);
\]

\[
W = 2.65/26;
\]

\[
\text{xRangeL} = \text{length(xRange)};
\]

\[
\text{estimate} = \text{zeros(length(xRange),1)};
\]

\[
\%Preallocating for speed
\]

\[
\text{PsiXrange} = \text{interp1(Psi(:,1), Psi(:,2), xRange)};
\]

\[
\text{for } i = 1: \text{length(PsiXrange)}
\]

\[
\text{if isnan(PsiXrange(i)) == 1}
\]

\[
\text{PsiXrange(i) = 0};
\]

\[
\text{end}
\]

\[
delta = x0(1);
\]

\[
sigma = x0(2);
\]

\[
\psiStar = x0(3);
\]

\[
\%Calculates the Psi values at the wkhalf points we're interested in, zeros
\%the ones that are outside the range (i.e. no direct laser component)
\]

\[
Knorm = 1/(\text{sigma} * \text{sqrt}(2*\text{pi}))*W*delta;
\]

\[
\%Definition of a constant, to remove recalcuations in the loop
\]

\[
\text{for } i = 1: \text{xRangeL}
\]

\[
\%Initialises scattered laser light for this spatial location
\]

\[
\text{scattered} = Knorm*\text{sum(Psi(:,2), exp(-(xRange(i)-Psi(:,1))^2/(2*sigma^2))});
\]

\[
\%Scattered portion of laser light
\]

\[
\text{direct} = (1-delta)*\text{PsiXrange(i)};
\]

\[
\%Direct laser light - unscattered, spatially corresponding NPFD, basically
\]

\[
\text{estimate(i)} = (1/\psiStar)*(\text{direct+scattered});
\]

\[
\%Sums the two into the total output
\]

\[
\text{end}
\]

\[
\%Gets the values from the model
\]

\[
\text{obj} = \text{sum((estimate - PoPk(:,2)).^2)};
\]

\[
\%Gets our objective
\]

\[
\text{end}
\]

\[
\text{function [npfd, xRange] = brute20130326(delta, sigma, psiStar, xRange, a)}
\]

\[
\%This function will hopefully generate plots of the TEDDvsChen idea. It \%
\%asks for a range (xRange, in mm) you'd like a prediction for, and Psi, given \%
\%as \%
\%a single vector, (X values in the first column, corresponding Psi(X) in the \%
\%second) \%
\%It also asks for a sigma, delta and scaling factor, Psi*(0). \%
\%\%tldr; will return [scattered] Po/Pk given a range, Psi(x), sigma, delta and \%
\%Psi*(0).
if a == 'Y'
    Psi = dlmread('PsiY.txt');
    PoPk = dlmread('PoPKY.txt');
else
    Psi = dlmread('PsiX.txt');
    PoPk = dlmread('PoPKX.txt');
end
W = 2.65/26;
xRangeL = length(xRange);
xRange = transpose(xRange);
estimate = zeros(xRangeL,1); directPlot = estimate; scatteredPlot = estimate;
%Preallocating for speed
PsiXrange = interp1(Psi(:,1),Psi(:,2),xRange);
for i=1:length(PsiXrange)
    if isnan(PsiXrange(i)) == 1
        PsiXrange(i) = 0;
    end
end
%Calculates the Psi values at the wkhalf points we're interested in, zeros
%the ones that are outside the range (i.e. no direct laser component)
Knorm = 1/(sigma*sqrt(2*pi))*W*delta;
%Definition of a constant, to remove recalculations in the loop
areaModel = 0;
for i=1:xRangeL
    %Initialises scattered laser light for this spatial location
    scattered = Knorm*sum(Psi(:,2).*exp(-(xRange(i)-
    Psi(:,1)).^2/(2*sigma^2)));
    %Scattered portion of laser light
    direct = (1-delta)*PsiXrange(i);
    %Direct laser light - unscattered, spatially corresponding NPFD,
basically
    estimate(i) = (1/psiStar)*(direct+scattered);
    directPlot(i) = (1/psiStar)*(direct);
    scatteredPlot(i) = (1/psiStar)*(scattered);
    %Sums the two into the total output
    areaModel = estimate(i)*(xRange(2)-xRange(1))+areaModel;
end
npfd = estimate*psiStar;
directPlotN = directPlot*psiStar;
scatteredPlotN = scatteredPlot*psiStar;

subplot(3,1,1), plot(PoPk(:,1),PoPk(:,2),'ro',xRange,estimate,'b*')
Legend('Experimental','Modelled')
xlabel('Length (mm)')
ylabel('PoPk')
title('TEDD-Chen Model vs Experiment')

subplot(2,1,2),
plot(xRange,directPlotN,'g+',xRange,scatteredPlotN,'m+',xRange,npfd,'b*')
Legend('Direct','Scattered','NPFD')
xlabel('Length (mm)')
ylabel('NPFD (1/mm)')
title('TEDD-Chen Model Components, Normalised')
areaModel
end
%Plots result, with a comparison to your Po/Pk (if provided)
Appendix D

The script presented here outlines the “brute force” method described in Section 5.2. It calls on a function “laserpropobj.m”, which is the code laserprop.m listed in Appendix A, modified to return the $R^2$ value between the simulation and experimental distributions, as well as the estimated transmission.

```matlab
%This program cycles through a number of simulations, calling
%LaserPropObjCreator for a massive number of combinations of variables. The
%idea is that the user can then look at the output, Solutions2.txt, and
%locate the values of transmission with the smallest obj values. Unlike the
%others, there is no "intelligence" - fmincon is not used. This is
%brute-force.
clear all
close all
% TEDDChenVarEstimatorY
% TEDDChenVarEstimatorX
% LM_BPD_Proc_2013mar13gzap
clear all
close all
global transmission
x0 = [0.5 0 1];
g0 = 0.04;
mua0 = 0.02;
mus0 = 0.3;
Solutions = zeros(1920,7);
a = 1;
t1 = 2.2;
t3 = 3.1;
tic
for i=1:12
    x0(1) = x0(1)+g0;
    x0(2) = 0.01;
    x0(3) = 0;
    for j=1:8
        x0(2) = x0(2)+mua0;
        x0(3) = 0.3;
        for k=1:20
            x0(3)=x0(3)+mus0;
            [A_rss1X trans1 A_rss2X trans2] = laserpropobj(x0,t1,t2);
            Solutions(a,1)=x0(1);
            Solutions(a,2)=x0(2);
            Solutions(a,3)=x0(3);
            Solutions(a,4)=transmission;
            Solutions(a,5)=A_rss1X;
            Solutions(a,6)=trans2;
            Solutions(a,7)=A_rss2X;
            fprintf('Iter = %d \n',a)
            if i==1
                toc
```
end
a=a+1;
end
dlmwrite('Solutions3_2mmUp_PCXXXX,XXmm.txt',Solutions);
end
toc
Appendix E

Parts of the solutions files produced by the brute force code listed in Appendix D are presented here.

PA-6

Table 0-1 Portion of brute force data for PA-6

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Table 0-2 Portion of brute force data for PC30GF

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