Feasibility Assessment of Compliant Polymers in TKR

by

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A thesis submitted to the Department of Mechanical and Materials Engineering in conformity with the requirements for the degree of Master of Science in Engineering

Queen’s University
Kingston, Ontario, Canada
August 2009

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Abstract

Total knee joint replacements (TKRs) are a commonly used treatment when joint pain becomes a major issue and the function of activities of daily living is impaired. TKRs may last for up to 20 years; however, younger and physically more active patients are receiving TKRs, necessitating increased prosthesis life-time. There has been considerable interest in more cartilage-like materials for the tibial inlay of a TKR. Compliant, rubbery polymers may be a first step towards such a material.

In this thesis, finite element analysis (FEA) was utilized to assess the feasibility of polycarbonate urethane (PCU) in a TKR application. Mechanical characterisation of PCU55D and PCU80A was performed in order to better understand the deformation behaviour of these materials. Mechanical test data was then used to tune and validate a hyperelastic material model. In a last step, the material model was applied to a static FE knee model which was used to simulate five discrete loading cases: three gait cycle events, stair climbing and squatting. Contact pressure, contact area and von Mises stress of the PCU inlay were compared to literature and to a standard ultra-high molecular weight polyethylene (UHMWPE) inlay.

The contact area of the articulating implant surfaces was on average 345% greater in PCU than in UHMWPE and contact pressure was on average 77% lower in PCU than in UHMWPE. The difference between TKRs simulated with a PCU tibial inlay and those simulated with a UHMWPE inlay increased with increasing flexion angle. The contact
pressures measured in TKRs simulated with a PCU tibial inlay were well below values that are expected to cause damage to the polymer, possibly reducing the risk of wear. The contact areas found in TKRs simulated with a PCU tibial inlay were close to what has been reported for the natural knee.

Considering the low contact pressures even at high flexion angles, where initial congruency is limited, it may be feasible to design less conforming knee prostheses that still exhibit low contact pressures, allowing for a greater range of motion. The reported results strongly indicate that compliant polymers may offer an opportunity to improve current TKRs.
Acknowledgments

First of all, I would like to extend my gratitude to my supervisor, Professor Urs Wyss, who has provided this great opportunity to study in Canada. I had always dreamed of studying abroad, and without Urs, it would most likely never have happened. Thanks a lot for your support.

To Ben Alcock, who has offered invaluable advice and guidance during the last year. Thanks for reading and improving my report! Ben was always prompt in responding to emails and always agreed to talk on the phone when something needed to be discussed. I really appreciate all the help and advice I have received from you.

A big thank goes to Adam Henderson for his Abaqus server support, to Eik Siggelkow and Marc Muenchinger who helped with Abaqus and the FE knee model, and to Giampaolo Franzoso for his invaluable UMAT, tensor algebra and Latex expertise. A thank also goes to Cornelia Steiger for her help with mechanical testing. I would also like to thank Joern Seebeck for his time during the initial phase of the project. Thank-you, Jeff Bischoff and Brian Thomas for your advice and support, especially during the time while I was in Warsaw.

I would also like to acknowledge the help and moral support I have received from the Biomech Group at Queen’s. I have made great friends here and I really hope that we will see each other again at some point! Simon, thanks a lot for your help with Matlab and Stacey, thanks for providing me with experimental data and for letting me use your text books. To my roommates, thanks a lot for your moral support during the last months. I
am fortunate to be your friend!

I would like to thank my family for their love and support during this great adventure! Without you, this would not have been possible!

Lastly, financial support by Zimmer GmbH and Queen’s University is gratefully acknowledged.
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Chapter 1

Introduction

1.1 Motivation and Objectives

Total knee joint replacements (TKRs) may be used when joint pain becomes a major issue and when functionality in the activities of daily living are severely impaired and no other treatment helps. One major cause of pain and impaired functionality is osteoarthritis (OA), which describes a progressive degeneration and loss of (hyaline) articular cartilage in synovial joints. OA is irreversible and therefore the damage caused is permanent.

TKRs have been successfully employed for many years and survival rates of up to 20 years have been reported. Replacing a knee joint with an artificial system is a relatively common operation with 602,600 procedures performed in 2007 in the United States alone. State of the art TKRs typically consist of three to four components: a metal tibial tray, a metal femoral component, a polymer tibial inlay and in some cases a patellar component. The metallic tibial tray substitutes the tibial plateau and the metallic femoral component replaces the femoral condyles, while the polymeric tibial inlay is placed between these two components, providing an articulating surface. The tibial inlay is most commonly made from ultra-high molecular weight polyethylene (UHMWPE).

TKRs are increasingly also implanted into younger patients, who may live a more active
CHAPTER 1. INTRODUCTION

lifestyle and have a longer life-expectancy when they receive the implant than the typical older TKR patient. Younger patients are likely to want to return to perform higher demanding physical activities after surgery and it would be desirable if revision due to limited implant lifetime could be avoided. Younger patients also tend to perform activities requiring a higher range of motion (ROM). Higher flexion activities inevitably lead to low contact areas between the femoral component and the tibial inlay, which combined with high knee loads, will significantly increase the stress on the tibial inlay, potentially exceeding the compressive yield strength of UHMWPE (8-15MPa).

There has been considerable interest during the last few years in developing artificial joints which more closely resemble the natural joint by using cartilage-like materials. It has been recognized that using compliant polymers with stiffnesses much lower than UHMWPE could be a first step towards developing such a TKR. By employing a compliant rubbery polymer, better load distribution may be achieved even with initially less congruent designs which would allow for higher range of motion. The use of compliant polymers may result in a better distribution of contact stresses and therefore have the potential to ultimately increase the life-time of a TKR.

The main objective of this thesis was to assess a compliant polymer for the use in TKR with the help of finite element analysis (FEA) using Abaqus (Version 6.8-1, Dassault Systèmes Simulia Corp., Providence, Rhode Island). In order to achieve this objective, the work was divided into three parts. After deciding which material to investigate, the material was mechanically characterized to determine its deformation behaviour. This provided test data that was then used to tune a constitutive equation applied in a finite element (FE) material model that is able to predict the desired deformation behaviour. After validating the material model by simulating certain experiments, it was used in an FE knee model with a TKR which simulates joint movement up to high-flexion. Typical knee loadings were simulated using the knee model. The performance of the compliant polymer was compared to the outcome of simulations using a UHMWPE inlay.
1.2 Thesis Outline

In Chapter 2, an extensive literature review containing general knee anatomy, OA background, TKR concepts, compliant polymer background, FEA theory and computational modeling of TKR background is presented. The next chapter, Chapter 3, introduces the various methods used for the experimental testing, material modeling development and FE knee modeling. In Chapter 4, the results are summarized according to the three subtasks of mechanical testing, material modeling and FE knee modeling. These results are discussed in Chapter 5 in accordance with these three subtasks and finally, in Chapter 6, the findings of the work are briefly summarized and recommendations for future work given. A summary of the work is provided in Chapter 7.
Chapter 2

Literature Review

In this chapter, some basic background information is going to be presented. Basic human knee anatomy followed by a brief description of osteoarthritis will be presented first. An overview of available total knee replacement designs will then be given. Next, a summary of compliant polymers in total joint replacements will be presented, followed by some background information on the candidate polymer, polycarbonate urethane (PCU). Lastly, basic FEA theory, constitutive modeling of elastomers and computational modeling in total knee replacements will be described.

Some basic anatomy of the human knee will now be discussed.

2.1 Anatomy of the Human Knee

In this section, basic anatomical terms, the main structure of the knee, kinematics and kinetics and lastly, lubrication of the human knee joint will be presented.

2.1.1 Anatomical Terminology

In anatomy, a unique vocabulary is used to describe locations within the body and to compare parts of the body with each other [3]. Tables 2.1 and 2.2 describe the most
important terms, and Figures 2.1 and 2.2 show visual representations of these terms.

Table 2.1: Anatomical planes of the body

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<th>Description</th>
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</thead>
<tbody>
<tr>
<td>Median Plane</td>
<td>vertical plane passing longitudinally through centre of the body - divides body in left and right halves</td>
</tr>
<tr>
<td>Sagittal Planes</td>
<td>vertical plane passing through the body parallel to median plane</td>
</tr>
<tr>
<td>Frontal or Coronal Planes</td>
<td>vertical planes passing through body normal to median plane - divide body into anterior and posterior halves</td>
</tr>
<tr>
<td>Horizontal or Transverse planes</td>
<td>horizontal planes passing through body normal to median and frontal planes</td>
</tr>
</tbody>
</table>

2.1.2 Main Structure of the Knee

The knee, a synovial joint, is the largest and most complicated joint of the human body. A joint is called a synovial joint, when the two bones forming it are separated by a joint cavity containing synovial fluid but are connected by a joint capsule. Synovial joints are the most important and common joints in the human body [3] and their main functions include permitting limited movement and transferring forces from one bone to another [16].

The knee joint is composed of three bones: the femur (thigh bone), the tibia (shin bone), and the patella (kneecap). Figures 2.3 and 2.4 show illustrations of the joint. The knee is basically composed of three separate joints, the femoropatellar joint, consisting of the patella and the patellar groove of the femur, the medial tibiofemoral joint, consisting of the medial femoral and tibial condyles, and the lateral tibiofemoral joint, consisting of the lateral tibial and femoral condyles (see Figure 2.3) [4]. The convex and asymmetric condyles of the femur are located at the distal end of the femur (see Figure 2.3 and Table
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Figure 2.1: Planes of the body, adapted from Moore et al. [3]

Figure 2.2: Terms for rotation and orientation, adapted from Netter [4]
Table 2.2: Anatomical terms of location and movement

<table>
<thead>
<tr>
<th>Term</th>
<th>Description</th>
<th>Term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proximal</td>
<td>closer to trunk or point of origin</td>
<td>Distal</td>
<td>further to trunk or point of origin</td>
</tr>
<tr>
<td>Anterior (ventral)</td>
<td>the front</td>
<td>Posterior (dorsal)</td>
<td>the back or behind</td>
</tr>
<tr>
<td>Medial</td>
<td>towards the median plane</td>
<td>Lateral</td>
<td>away from the median plane</td>
</tr>
<tr>
<td>Flexion</td>
<td>decreasing angle between two segments or bending</td>
<td>Extension</td>
<td>straightening a segment or increasing angle</td>
</tr>
<tr>
<td></td>
<td>of a segment</td>
<td></td>
<td>between two segments</td>
</tr>
<tr>
<td>Adduction</td>
<td>moving segments towards median plane in frontal</td>
<td>Abduction</td>
<td>moving segments away from median plane in frontal</td>
</tr>
<tr>
<td></td>
<td>plane</td>
<td></td>
<td>plane</td>
</tr>
<tr>
<td>Internal Rotation</td>
<td>inward rotation of segment along its long axis</td>
<td>External Rotation</td>
<td>outward rotation of segment along its long axis</td>
</tr>
</tbody>
</table>

(a) Anterior view of flexed knee joint with ligaments
(b) Posterior view of knee joint with ligaments

Figure 2.3: Right knee joint with soft tissue removed, adapted from Netter [4]
Figure 2.4: Sagittal section cut of knee joint, adapted from Netter [4]
2.2), whereas the concave, asymmetric articulating surfaces of the tibia are located at the proximal end of the tibia (see Figure 2.3 and Table 2.2).

The tibiofemoral joint is often described as a modified hinge joint which, apart from the primary motion of flexion and extension in the sagittal plane also allows anterior-posterior (AP) gliding, rolling, small amounts of abduction and adduction in the frontal plane (see Figures 2.1 and 2.2 and Tables 2.1 and 2.2), and rotation about a vertical long axis [3, 17]. Due to the fact that the knee lacks bony protrusions to limit the range of motion, its stability depends on ligaments connecting the femur and tibia, muscles and their tendons [17]. Muscles are the most important stabilizers [3] with the quadriceps femoris being the main muscle which stabilizes the knee (see Figure 2.5(a)). There are two main muscle groups responsible for flexion and extension of the knee, the aforementioned quadriceps femoris and the hamstrings, which include the semitendinosus, semimembranosus, and the bicep femoris (see Figure 2.5). The contraction of the quadriceps causes extension of the knee while the contraction of the hamstrings causes flexion of the knee [18]. Two main ligament systems are present at the knee as can be seen in Figure 2.3, the collateral ligaments and the cruciate ligaments. The anterior and posterior cruciate ligaments (ACL and PCL) are named after their tibial attachment; the ACL originates at the anterior surface of the tibia and the PCL is attached to the posterior side of the tibia. The ACL extends to the posterior side of the femur while the PCL extends to the anterior side of the femur. These two cruciate ligaments provide rotary and anterior-posterior (AP) stability and their passive tension prevents the femur from sliding off the tibia or vice versa [17]. The second set of ligaments, the medial and lateral collateral ligaments (MCL, LCL), provide medial-lateral (ML) stability. The MCL is, to some extent, connected to the capsular fibres and the medial meniscus. Conversely, the LCL is not attached to either the capsule or the meniscus [17]. The collateral ligaments mainly stabilize the extended knee while the cruciate ligaments are responsible for the stability of the flexed knee.

The areas of the tibia, femur and patella which are part of the joint are covered with
(a) Quadriceps femoris from anterior side - Superficial layer (Vastus intermedius not visible)

(b) Biceps femoris, semitendinosus and gastrocnemii from posterior side

(c) Semimembranosus and gastrocnemii from posterior side (Biceps femoris and semitendinosus partly removed)

Figure 2.5: Important muscles acting at the knee, adapted from Sobotta [5]
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Articular cartilage (see Figure 2.4), which acts as a gliding surface with very low coefficient of friction (see Section 2.1.4) [3]. Articular cartilage is a layer of fibrous connective tissue with a large water content. Some of the main functions of articular cartilage are: reducing joint friction during movement, distributing forces, and transferring forces [16].

The tibia and femur are separated by two asymmetric, wedge-shaped, fibrocartilaginous discs called menisci (see Figures 2.3 and 2.4) [17]. The lateral of the two is only loosely connected to its surroundings and therefore allowed to move freely. It has a circular or ring shape. The C-shaped medial meniscus, on the other hand, is firmly attached to its surrounding and therefore restricted in its motion [17]. The menisci increase the contact area (congruency) in the joint by deforming under load, hence spreading out the forces transmitted through the knee. This is important because it protects the articular cartilage from excessive point loads and therefore minimizes the risk of damage of the cartilage. It is estimated that approximately 40 to 60% of the compressive load transferred through the knee joint is carried by the menisci. Menisci also act as shock absorbers and provide some ML stability when the knee is fully extended [17].

The patella, which is part of the femoropatellar joint, is attached to the quadriceps tendon and is connected to the tuberositas tibiae (see Figure 2.4) through the patellar tendon. The patella ensures that the attack angle of tendon at the tuberositas tibiae is always optimal (see Figure 2.6) [4] and its main function is to increase the moment arm of the quadriceps [17].

The knee joint is enclosed with the articular capsule, the synovial membrane that seals the joint and is interconnected with the ligaments. The space within the capsule, the joint cavity (see Figure 2.4), which is the largest cavity in the body [3, 4], is filled with synovial fluid which acts as a lubricant.
2.1.3 Kinematics and Kinetics

As mentioned in section 2.1.2, the tibiofemoral joint does not possess any bony restrictions to movement, and so the ligaments and the joint capsule determine the range of motion [17]. The American Academy of Orthopaedic Surgeons reported that if a joint angle of 0° implies that tibia and femur are parallel, the passive range of motion of a healthy human knee is from -10° (hyperextension) to 134° (full flexion), resulting in a total excursion of 144° [19]. Several studies reported average extension-flexion angles for the knee joint during an entire gait cycle of level walking ranging from 1.5° to 66.7° [1, 7, 14]. Usually, the knee is flexed during the entire gait cycle; however, hyperextension of up to -8° has been reported [1]. A gait cycle is usually expressed in percentage and is divided into stance period and swing period, where the former normally constitutes 60% of the cycle and the latter 40%. A gait cycle starts with the first phase of the stance period, the heel strike, and ends with the last phase of the swing period, terminal stance or heel strike of the same leg (see Figure 2.7). The stance and swing periods are further split into five and three phases, respectively. The stance phase consists of the heel strike, loading response, mid stance, terminal stance and
Table 2.3: Average knee flexion angles during activities of daily life, adapted from Rowe et al. and Hemmerich et al.[1, 2]

<table>
<thead>
<tr>
<th>Description</th>
<th>Min Angle [°]</th>
<th>Max Angle [°]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Level Walking</td>
<td>1.5</td>
<td>66.7</td>
<td>[1]</td>
</tr>
<tr>
<td>Downhill Walking</td>
<td>3</td>
<td>70</td>
<td>[1]</td>
</tr>
<tr>
<td>Uphill Walking</td>
<td>1.1</td>
<td>63</td>
<td>[1]</td>
</tr>
<tr>
<td>Upstairs Walking</td>
<td>16.7</td>
<td>94.1</td>
<td>[1]</td>
</tr>
<tr>
<td>Downstairs Walking</td>
<td>17</td>
<td>93.9</td>
<td>[1]</td>
</tr>
<tr>
<td>Sitting Down on Standard Chair</td>
<td>6.5</td>
<td>96.7</td>
<td>[1]</td>
</tr>
<tr>
<td>Squatting</td>
<td>-</td>
<td>156.9</td>
<td>[2]</td>
</tr>
<tr>
<td>Kneeling</td>
<td>-</td>
<td>154.9</td>
<td>[2]</td>
</tr>
</tbody>
</table>

pre swing, where as the swing phase is initiated by toe off, when the toes leave the ground, followed by mid swing and terminal swing or heel strike of the same leg [6]. Figure 2.8 shows an illustration of the knee flexion angle during an entire gait cycle. One can see that the flexion angle is at maximum during initial and mid swing (at 70% of gait cycle).

In a study from 2000 performed by Rowe et al. [1], flexion angles for the knee during activities of daily life, such as level walking, uphill and downhill walking, and sitting down on a chair, were reported for elderly subjects (mean age 67). Their findings are summarized in Table 2.3. Recently, there has been an interest in activities of daily living that require flexion angles of 140 to 150°. Such activities include squatting and kneeling, which are very common in some cultures. High flexion angles in the knee are particular relevant in the younger population because more dynamic activities are expected. Hemmerich et al. have measured three dimensional kinematics of hip, knee and ankle joint during high range of motion activities in 30 Indian subjects [2]. The maximum flexion angles at the knee were found to be between 153.7 and 156.9° for squatting and 144.4 to 154.9° for kneeling. Table 2.3 reports the minimum and maximum values of flexion which were measured in the above studies.

The amount of possible internal and external rotation (see Figure 2.2) of the knee is dependent on the flexion angle. At full extension, the ligaments are taut and the knee is
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Figure 2.7: Different events of the gait cycle, adapted from Rose et al. [6]

Figure 2.8: Knee flexion and extension angle during level walking from heel strike to heel strike (0-100%), adapted from Kadaba et al.[7]
in its most stable position. In this locked position, no rotation is possible [17] and the leg is able to support the body weight despite the quadriceps being relaxed. The mean range of internal and external rotation during gait is approximately $9^\circ$ [20]. Abduction and adduction of the knee (see Figure 2.2) is very limited and may only be invoked passively. Slight abduction and adduction may also occur during walking [17].

The knee joint is subject to high compressive forces during activities such as walking, running and stair climbing. Many research groups [20–28] have investigated forces and moments occurring at the knee. They use common techniques including combinations of video motion analysis (gait analysis) and force plate measurements to calculate forces and moments using inverse dynamics and computer models. Some groups use instrumented total joint replacements to measure forces directly [22, 24, 29, 30]. Depending on the activity, axial compression forces at the knee differ widely. A reasonable range for activities of daily life is 1-5 times body weight, where low forces occur during level walking and higher forces at high flexion activities, where the contact area is lower, as will be discussed in Chapter 5. Generally, there is high congruency at low flexion angles and low congruency at high flexion angles greater than $80^\circ$.

### 2.1.4 Lubrication of the Human Knee Joint

When describing lubrication regimes in joints, different terms are used: full fluid lubrication (hydrostatic and hydrodynamic), elastohydrodynamic lubrication (EHL), squeeze film lubrication, boundary lubrication, and mixed lubrication. These will now be defined. Fluid film lubrication occurs when asperities of contact areas are completely separated by a fluid film. In hydrodynamic lubrication, the contact surfaces are rigid enough to prevent significant deformation and the lubricant is drawn into a gap between the two surfaces by their respective motion while in hydrostatic lubrication contact surfaces are held apart by the lubricant which is injected under pressure. Elastohydrodynamic lubrication (EHL) is a thin film lubrication in which the lubricant film becomes too thin to completely separate the two
surfaces in contact. EHL occurs when the bearing material is relatively soft, for example in cartilage, permitting deformation. The deformations of the soft contact surfaces, which are large with respect to the film thickness, increase the contact area and this decreases the pressure in the film and increases the minimum thickness of the film. Squeeze film lubrication is a special class of hydrostatic lubrication where the film persists for a certain amount of time after relative motion of the contact surfaces has stopped. Boundary lubrication is dependent on chemical rather than physical properties of the lubricant and the film covering the articulating surfaces is very thin. In mixed lubrication, the load is carried partly by boundary lubrication and partly by fluid films [31].

Natural synovial joints have been shown to mostly operate in a fluid film regime, where the two contact areas are predominantly separated by a fluid film [31–35]. The fluid film lubrication is achieved by a combination of full fluid film, elastohydrodynamic, microelasto-hydrodynamic and squeeze film lubrication [8, 32, 34, 35]. In the hip and the knee during the lightly loaded swing phase, full fluid film prevails. At heel strike and toe off, during which the two joints are subject to relatively short bursts of very high loads, squeeze film lubrication is present, where the prior established fluid film thickness is reduced because the liquid is squeezed out of the joint space. During the stance phase, EHL is the dominant mechanism [8, 35]. After an extended period of motionlessness (for example resting or standing) when the joint is again moved, the potential for wear is high due to the articular surface contact. However, a boundary lubricant is present that keeps the friction low and therefore helps to protect the cartilage [36]. The fluid film between the articular surfaces provides lubrication whenever it can support the applied load. When the loads are too high and the velocity too low, a boundary lubricant plays a major role [36]. Coefficients of friction (COFs) for the human joint have been reported to range from 0.002 to 0.04 [20]. Figure 2.9 illustrates the aforementioned gait events with their respective lubrication regime.
Figure 2.9: Lubrication of hip joint at different gait events, adapted from Isenberg et al. [8]
Because osteoarthritis is such a major cause of joint function impairment, a brief description of how it effects joint articulation is now presented.

2.2 Osteoarthritis

Osteoarthritis (OA), which is among the most prevalent chronic diseases in the world, is the most common joint disease (see Figure 2.10). Worldwide, it is among the leading causes for pain and (long-term) disability [37]. The disease describes the progressive degeneration and loss of (hyaline) articular cartilage in synovial joints, which is accompanied by hypertrophy (osteophyte activity and subchondral bone sclerosis) of the surrounding bone and thickening of the joint capsule. Symptoms include joint pain, local inflammation, decreasing range of motion which lead to muscle atrophy, morning stiffness and swollen joints. Symptoms can be alleviated, but the progression of the disease can not yet be stopped. Any joint can be affected by OA; however, the hip, knee, wrist and lower back are the most affected joints [38]. Two types of OA can be distinguished: primary OA is a chronic disease and is usually seen in weight bearing joints, such as the knee or hip, while secondary OA is due to other arthropathies or secondary to trauma [39, 40].

All ethnic groups in all geographic regions are affected by OA. Both men and women are affected, but overall women are commonly more affected. More than 33% of the people over the age of 45 report occasional joint stiffness and intermittent aching related to activity [41]. A study performed in 2000 for The World Health Organization (WHO) reported that approximately 10% of the world population over the age of 60 have OA [42]. In some populations, over three quarters of the population over the age of 65 are reported to suffer from OA in one or more joint [41]. It is estimated that about 9.6% of men and 18% of women worldwide have osteoarthritis (see Figure 2.11) [38]. The prevalence of OA increases with age, which is the most evident predictor of the development and progression of radiographic OA [42]. Obesity is another risk factor that leads to OA, especially of the
Figure 2.10: Osteoarthritis of femur and patella, adapted from Netter [4]. The rough surfaces of the patella and femur illustrate degeneration of the cartilage.
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Figure 2.11: Percentage of the male and female population affected by OA

hand, knee and the hip [43]. Other risk factors for the development of knee and hip OA include trauma and certain physically demanding activities [44]. There are only few data published on the incidence of OA, since it is difficult to define and determine the outbreak of the disease. Since the incidence of OA correlates with age, and because life expectancy is increasing, it is thought that OA will become the fourth leading cause of disability by the year 2020 [38].

OA has been ranked as a main worldwide cause of economic loss [41]. In 2002 J.Y. Reginster [45] reported that the economic burden of OA accounts for 1-2.5% of the gross national product of western countries. This burden includes direct cost of medical intervention and indirect costs, such as early death and chronic and short-term disability. In the U.S. alone, it was estimated that OA costs more than USD 60 billion per year [41].

There are two approaches to treat OA, nonsurgical treatments and surgical intervention. The former can include lifestyle changes, where high-impact activities may be substituted
with low-impact activities in order to reduce pain, medication (anti-inflammatory) to help decrease pain and therapy including ice or heat treatment, supportive devices and physical and/or occupational therapy. Surgical treatment may include arthroscopy (localized treatment), realignment of bones to reduce pressure on the effected joint (osteotomy), joint replacements and ultimately joint fusion [46]. The most common surgical treatment to treat OA, total knee replacements, will be discussed next.

2.3 Total Knee Replacements

In this section, the basic concept of total knee replacements, followed by some design limitations of common total knee replacements will be presented.

2.3.1 Basic Concept

The main reasons for receiving a total knee replacement (TKR) are pain and limited functionality due to decreased range of motion, but pain is the most important factor. There are numerous different types of TKRs on the market. However, many designs consist of a polymer component between two metal components (see Figure 2.12). The distal end of the femur is replaced by a metal femoral component, which resembles the femoral condyles, whereas the proximal tibial end is replaced by a metal tibial tray which accommodates the polymer tibial inlay. Figure 2.12(a) shows a possible configuration of a conventional TKR. Depending on the severity of the knee joint defect, either both compartments (medial and lateral) or just one compartment may be replaced (see Figure 2.12(b)). In some cases, the articulating surface of the patella is also replaced by a full polymer part (see Figure 2.13(b)) or a polymer articular surface with a metal backing (see Figure 2.13(a)). The tibial insert is usually made from ultra high molecular weight polyethylene (UHMWPE), while the femoral and tibial components are commonly made from a titanium (Ti) or cobalt-chrome (CoCr) alloy. A few designs consist only of a metal femoral component and a UHMWPE tibial
component in which the tray and the inlay are one piece (see Figure 2.14(a)).

There are basically two concepts regarding fixation of orthopaedic prostheses: cemented and cementless. For the former, a bone cement layer connects the implant (tray and femoral component) to the bone, while in the latter the implant components are in direct contact with the bone. In cementless implants, primary stability is achieved by press fit and secondary stability is gained by encouraging bony ingrowth. In order to achieve ingrowth, the implant surfaces are rough with holes and depressions where the bone can bond to the implant (see Figure 2.15). Two different approaches may be employed for the tibial insert: a mobile insert, where the insert is to a certain extent able to slide on the tibial tray, and a fixed approach, where the inlay firmly clips into the tray. For the fixation of the tibial tray two different designs are employed, one with a central stem (see Figure 2.16(a)) and a pegged design (see Figure 2.16(b)). Another design aspect that distinguishes TKRs is the role of the PCL, which among other things, restrains the posterior motion of the tibia in relation to the femur. The ligament is either retained or sacrificed and usually substituted
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(a) Patella replacement

(b) Full polymer patella replacement

Figure 2.13: Patella replacement designs, ©Zimmer GmbH

by a polymer post (see Figure 2.14(b)).

According to a review by Mendenhall [47] from 2008, a total of 602,600 TKR procedures were performed in 2007 in the US alone, of which 506,200 were primary total knee replacements, 47,800 primary unicondylar knees and 48,600 revision surgeries. In comparison, 423,050 hip replacements were performed. More than a quarter (28.8%) of all knee replacements sold in 2008 were Zimmer products, giving the company the largest market share. According to a 2009 survey conducted by Mendenhall [48], the typical cost of a bi-condylar TKR is between 9,362 and USD 12,224 while unicondylar knee replacements cost USD 6,066.

2.3.2 Design Limitations of Common TKRs

As discussed in section 2.3.1, conventional artificial joints often consist of a UHMWPE component between two metal components. UHMWPE has been employed in total joint replacements (TJRs) for the past 40 years [49] and post-operative follow-up studies of patients have shown that TKRs can survive for up to 20 years [50] and total hip replacements (THR) for up to 25 years [51]. Nevertheless, orthopaedic prostheses have a finite life and
(a) Full polymer inlay and tray

(b) Inlay with post substituting PCL

Figure 2.14: Examples of tibial inlay designs, ©Zimmer GmbH

Figure 2.15: Femoral component with porous surface, ©Zimmer GmbH
are now being implanted in younger patients that have a more active lifestyle and longer life-expectancy. It is therefore desirable to increase the life-time of total joint replacements.

There are several failure modes which can necessitate revision or replacement of an orthopaedic implant. However, the majority of the failures are due to late aseptic loosening [52, 53]. One of the most common explanations for aseptic loosening is periprosthetic osteolysis, which describes the resorption of bone surrounding the implant [54]. Bone resorption may in turn lead to implant loosening and ultimately implant failure. It is more and more accepted that osteolysis is due to wear particles, especially particles from UHMWPE [54–57]. Wear can only occur when two articulating surfaces are in direct contact with each other. Studies have shown that TJRs operate in boundary or mixed lubrication regime, where the load is carried partly by boundary and partly by a fluid film (see section 2.1.4) [58–63]. Mixed lubrication inevitably leads to material contact and therefore potential wear. It has been shown that some of the factors contributing to osteolysis are the particle size, number of particles and the rate at which particles are generated [64, 65]. It is not the total wear volume that triggers osteolysis, but the concentration of wear particles of critical size,
which has been found to range between 0.1-1.0μm [56, 57]. As described earlier, osteolysis is a major reason for total hip replacement revision and makes reconstruction significantly more difficult due to the fact that local bone is weakened [55]. Osteolysis seems to be less common in TKRs because wear particles are usually larger than those generated in THR, but it does occur [64, 66]. Apart from failures directly attributed to periprosthetic osteolysis, implants may also fail because of mechanical loosening of the components, implant failure and other mechanical problems. However, some of these problems might be additional consequences of wear and osteolysis [64].

To target TKRs at younger, more active patients, it is advantageous to have increased post-operative range of motion (ROM). Additionally, such patients are likely to participate in more physically demanding activities such as playing tennis, cycling and down hill skiing, increasing the mechanical stress applied to the TKR. High-flexion activities such as squatting or kneeling have been shown to result in high knee loads (see section 2.1.3) but also likely to result in reduced contact area. The combination of higher loads and lower contact area significantly increases the stress on the joint replacement, often exceeding the compressive yield strength of UHMWPE (8-15MPa).

In this section, it was shown that current TKR designs are generally successful but at the same time, when targeting a younger and more active population, improvements need to be made. In the following section a possible way to improve current TKRs will be proposed.

2.4 Compliant Polymers

One possible way to improve current TKR designs is to use more compliant polymer materials for the tibial inlay. Such a material necessarily needs to be a biomaterial, which, according to Williams, describes a material that has the ability to exist with human tissue without causing an unacceptable degree of harm to the body [67].

One of the ideas behind using compliant materials for joint replacements is to more
closely mimic the low elasticity of articular cartilage, which could promote full fluid film lubrication, as it is found in natural joints (see Section 2.1.4), and therefore possibly reduce wear [62, 68].

In the artificial knee, requirements for biomechanics and tribology demand conflicting properties [69]. While from a biomechanical viewpoint only limited conformity and therefore a small contact area is desired in order to achieve large range of motion, while from a tribological and structural perspective a large contact area is necessary in order to reduce contact stresses [62] and therefore potential damage to the articular surface. This is one area in which compliant polymers could offer an alternative solution. Due to the availabilities of different compliant polymers with a wide range stiffnesses, it may be possible to design less conforming knee implants which could increase the range of motion but still provide enough contact area due to deformation and therefore lessen contact stress [69].

2.4.1 Friction, Wear and Lubrication - A review of in Vitro Studies

One of the earliest reports of the use of soft layers in artificial joints, specifically hip joints, was by Unsworth et al. in 1981 [70]. They found in functional hip simulator studies, using different lubricants, that when a soft silicon rubber is bonded either to the acetabular cup or to the femoral head of a Charnley type hip implant, coefficients of friction (COF) were lower than in the original Charnley joint and full fluid film lubrication is developed. Since then, several groups have investigated compliant polymers as an alternative material in TKRs [69, 71–78], THRs [59, 75, 77, 79–86], and shoulder implants [87]. Various groups have also examined wear and friction performance as well as biostability of compliant polymers [88–94].

Different compliant polymers have been considered as implant materials, such as silicone rubber, polyurethanes and other synthetic rubbers [85]. Full silicone implants have been used in the foot, elbow and wrist, although, early silicone devices often caused silicone synovites [95]. There has also been interest in hydrogels as compliant materials in medical
devices [96–99]. While hydrogels exhibit low friction and wear rates are relatively low, there are also problems such as durability and fixation associated with them. The majority of the work on compliant polymers has focused on polyurethanes (PU) due to their relatively good history in long-term medical applications, such as pacemaker lead insulation [91].

Various investigators have shown that compliant polymers have the potential to operate in full fluid film lubrication regime (see Section 2.1.4) and may therefore be less prone to wear. Lubrication regimes are often estimated using Strubeck plots that show the friction factor, $f$, as a function of the Sommerfeld number $Z$. The friction factor maybe obtained from simulator studies and is calculated from a frictional torque, $T$, applied load, $L$, and radius, $r$, of the femoral condyle (TKR) or femoral head (THR). The friction factor for hip joints is similar in magnitude to the COF [100]:

$$f = \frac{T}{rL} \quad (2.1)$$

The Sommerfeld number is a function of lubricant viscosity, $n$, entraining viscosity, $u$ and applied force, $L$:

$$Z = \frac{nu r}{L} \quad (2.2)$$

Due to the fact that the Sommerfeld number is a function of the lubricant viscosity, it is possible to predict the necessary viscosity to achieve full fluid film lubrication. A decreasing friction factor with increasing Sommerfeld number indicates mixed lubrication, while an increasing friction factor with increasing Sommerfeld number indicates full fluid film lubrication and a constant friction factor suggests boundary lubrication. In addition, a dimensionless parameter $\lambda$ is often calculated based on the root mean square surface roughness of the articular surfaces and a theoretical minimum film thickness, which is a function of viscosity, entraining velocity, compliant layer thickness, surface roughness, load and various modulus terms. A $\lambda > 3$ would predict full fluid film lubrication [101].

Auger et al., in 1993 [59], compared friction and lubrication of cushion form and
UHMWPE bearings using a pendulum hip simulator and found that using cushion form bearings improved lubrication, demonstrating strong evidence of full fluid film lubrication. In 1998, Bigsy et al. [84] conducted wear simulation for up to four million cycles using a hip simulator and compared PU surface damage and wear rate to conventional UHMWPE showing that the former performed better. Overall, their findings supported the idea that cushion joints can operate with full fluid film. Several other investigators measuring friction of PU in THR using dynamic friction hip simulations also showed that PU can outperform UHMWPE, by exhibiting lower friction factors and appearing to work in full fluid film regime rather than in mixed lubrication regime [79, 81, 82]. In 2003, Scholes et al. [68] compared the lubrication regime and friction behaviour of UHMWPE, PU compliant layer and hard bearing surfaces in THR. They conducted friction simulations on a hip simulator using different viscosity carboxymethyl cellulose (CMC) lubricants. CMC with certain viscosities have been shown to be similar to synovial fluid. Friction factors measured for PU ranged from 0.001-0.012 compared to 0.18-0.3 for hard metal bearings and 0.01-0.04 for metal- and ceramic-on-UHMWPE joints. Jones et al. in 2009, conducted dynamic friction simulation studies and fatigue tests using polycarbonate urethane (PCU) acetabular cups measuring friction factors ranging from 0.0005-0.025, which is slightly lower range than reported values for UHMWPE (0.015-0.035) [77]. Dynamic compression fatigue tests run for up to 14.4 million cycles did not reveal any visual damage or debonding of the cups.

Similar promising results have been found for TKRs in in vitro studies. One of the earliest investigations was performed by Auger et al. in 1995 [69] who used a pendulum simulator to examine the friction and lubrication performance of two simplified PU TKR models (cylindrical metal femoral component), one with an elastic modulus of 6MPa and one with an elastic modulus of 20MPa. Friction factors were found to range from 0.001-0.045, compared to 0.05-0.2 for UHMWPE. The more compliant PU exhibited less wear and friction than the stiffer PU. The analysis suggested mixed lubrication with a high percentage of full fluid film lubrication. In the same year, Auger et al. used the same type of implant
and materials with different layer thicknesses to investigate wear and creep performances. Tests were conducted in deionised water at room temperature and run until failure. It was found that the stiffer PU did not fail and was tested for up to 5 million cycles without any visible wear debris. The PU with an elastic modulus of 6MPa, however, failed after less than 200,000 cycles due to almost complete debonding of the soft layer from its substrate, resulting in substantial wear debris. The issue of debonding is further discussed in Section 2.4.4. The tests demonstrated that a compliant tibial bearing can be constructed so that it produces very little wear. In a more recent study from 2007, Scholes et al. [72] tested a PCU unicompartmental knee prosthesis on a wear simulator for 5 million cycles using bovine serum at 37°C. Post-wear simulation examinations did not reveal any surface damage. Wear rates of 1.12mm³/mio cycles were significantly lower than wear rates observed in UHMWPE (3.2 – 4.1mm³/mio cycles). Friction tests were conducted before and after the wear tests, applying a simple harmonic motion in the sagittal (flexion-extension) plane. Different viscosities of CMC lubricant and bovine serum were investigated. The analysis of the friction results indicated that the joints run in close to full fluid film lubrication. Also, friction factors were measured before and after wear simulation tests and were shown to be similar. The friction factors were reported to be 0.004-0.05 when CMC was used as lubricant and 0.04-0.1 when bovine serum was used as a lubricant. Some tests ran dry, significantly increasing wear and friction factors; however, the components were able to recover and wear and friction factors returned to values prior to running dry. In addition, the structure of the PCU component was reported to be unaffected. In 2008, Jones et al. [78] assessed the tribology and design of tibial inserts using two different types of PU (with different moduli) and UHMWPE. Friction factors were measured on a friction simulator applying a dynamic, oscillating load and lubrication regimes were determined. Different viscosity CMC lubricants were used and testing was performed at room temperature. PU was shown to give lower friction factors than UHMWPE and when manufactured to an appropriate design, full fluid film lubrication was achieved.
Several research groups have conducted friction and wear studies under adverse conditions. In 2004, Ash et al. [71] added bone cement particles to the articulating surfaces of a TKR using both UHMWPE and PCU while performing friction and wear tests. Distilled water with added bone cement particles was used as a lubricant. First, a friction test without particles was performed, followed by a three million cycle wear test with third body particles. After the wear experiment, another friction test was conducted. It was found that UHMWPE exhibited almost three times higher friction torque moments than PU (2,030Nm vs 742Nm). It was reported that adding the particles greatly increased the friction. Depending on the amount of particles introduced to the sample, the torque increased to 4,479Nm for PU and 10,073Nm for UHMWPE. PU torques were always lower than UHMWPE torques. Lubrication analysis using Stribeck plots indicated that UHMWPE operated in mixed lubrication whereas PU operated close to full fluid film lubrication. It was also found that particles firmly embedded in the UHMWPE but not in the PU components. A year earlier, in 2003, Jones et al. [75] had reported a similar study in which they had added bone cement particles to the articular surface of TKRs and THRs in vitro, measuring friction and wear for up to 6 million cycles. The measured frictional torques for PU were at least three times lower than for UHMWPE (1.5Nm vs 5Nm) and there was no visible damage to the PU articular surfaces, whereas in UHMWPE surface damage was visible. Also, PU was shown to operate in full fluid film lubrication. Similarly, Wang et al. [76] tested a compliant PU and a UHMWPE bearing surface for a TKR for nine million cycles with added bone cement particles. The results showed that the surface appearance of the compliant polymer did not change after the wear test and, unlike in UHMWPE, there were no embedded particles visible. UHMWPE also showed surface pitting after testing.

Although friction and wear studies by different researchers vary in terms of test conditions (lubrication, testing at room temperature, simplified designs, etc.) and there are not yet any longterm clinical results, there is still evidence that compliant polymers in TJR can perform better than UHMWPE and therefore may have improved life-time expectancy.
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The fact that friction and wear of compliant polymers as articulating surfaces in TJR simulations is often lower than UHMWPE articulating surfaces in TJR simulations is usually attributed to better lubrication mode, e.g. near full fluid film lubrication rather than mixed lubrication. It is believed that the low stiffness of compliant polymers allows EHL (see Section 2.1.4) in which the soft asperities of the articular surface can be deformed by the lubricant pressure and therefore enabling the maintenance of a thinner film thickness [69]. In addition, due to the low stiffness of these polymers, larger contact areas are possible without a conforming geometry, which reduces contact stresses [69].

2.4.2 Friction, Wear and Lubrication - A review of In Vivo Studies

In a study from 2004 by Khan et al. [80], THRs consisting of a scaled-down standard hip shaft based on the Exeter Hip by Stryker (Kalamazoo, Michigan) articulating against a PCU acetabular cup were implanted into 37 sheep for up to four years. A conventional THR with a UHMWPE cup was also used for a one year comparison, however no comparison to PCU was reported. After three years (no results were reported for the fourth year), soft tissue and organs were screened for abnormal responses and the bearing surfaces of the retrieved components were examined with electron microscopy. In addition, core samples were taken from the bearings and compared to control cores of virgin specimens to compare physiochemical properties. Wear was found to be minimal and no significant tissue damage, wear particles or inflammatory tissue responses were observed. Two years later, in 2006, Carbone et al. reported a similar study with an ovine hip arthroplasty model using PCU as a compliant layer acetabular cup [83]. 36 sheep were used, each assigned to a 6-month, 12-month, 24-month or 48-month group. Before sacrificing the animals, passive ROM was assessed in both the healthy and the THR hips. Possible acetabular cup loosening was assessed at retrieval, the synovial tissue was analyzed using light microscopy, and lymph node and tissue of the lung, kidney, liver, and spleen were examined for presence of wear particles and abnormal tissue response. Acetabular cups were also visually inspected for
significant wear or damage. No macroscopic evidence of wear or fractures was found in the compliant layers, e.g. no fractures, pitting, grooves or delamination. The author concluded that the almost complete absence of wear supports the idea that the joint operated in a full fluid film regime. Some specimens showed a low concentration of polymeric particles in the synovial tissue, where the incidence decreased with increasing implantation duration, with the 48-month group not showing any particles at all. The authors suggest that these particles are possibly due to smoothing of the asperities in the early post operative period. Electron microscopy would have been necessary to detect the presence of submicron particles, but based on the absence of significant inflammatory response in the local tissue, it was assumed that significant amounts of submicron particles were not present.

2.4.3 Some Design Aspects of Using Compliant Polymers in TKR

Several groups have looked at design aspects of compliant polymers. More highly compliant layers can neither be directly attached to the bone nor to a metal tibial tray. Hence, it is necessary to attach the more compliant layer to a stiffer base layer in order to make the prosthesis functional. Often the base layer is made from a stiffer polymer substrate with a more compliant layer on top of it, in which one the less stiff polymer is moulded over stiffer polymer [75–80, 82, 83].

In their 1995 TKR studies, Auger et al. [69, 74] investigated two different soft layer thicknesses, 2.5 and 5mm as well as polymers with two elastic moduli, 6 and 20MPa. In the friction studies, the material with stiffness of 6MPa was shown to exhibit lower friction than the material with stiffness of 20MPa. However, in the wear and fatigue study it was seen that the strength of the polymer with a stiffness of 6MPa was not sufficient, whereas the polymer with a stiffness of 20MPa worked for up to 5 million cycles. In 2008, Jones et al. investigated three different PCU tibial inlay conformities (low, medium and high) and three different thicknesses (2, 3 and 4mm) [78]. Two PUs with different elastic moduli, 19.2MPa and 37.9MPa were also analysed. Layer thickness and conformity were found to
have only little influence on friction. However, for optimal ROM, lowest contact stress and lowest impingement, it was concluded that a low to medium conformity bearing would be ideal. Overall, it was also concluded that an inlay with thickness of 2mm and a modulus of 19.2MPa with low to medium conformity was optimal in these tests. Jones et al. [77], in 2009 found in TKR wear studies that it was not suitable to use an inlay design which has been optimised for UHMWPE, for moulding PU inlays, because the difference between the material properties of UHMWPE and PCU means that, the functions of the inlay are completely different. Also, they found that a 2mm thick inlay performed better than a 3mm thick inlay.

2.4.4 Possible Issues with the Use of Compliant Polymers

A few potential issues with the use of compliant polymers in TJRs have been identified in literature. Although the COF of lubricated PU specimens is very low (see Sections 2.4.1 and 2.4.2), the COF of dry PU specimens is very high, significantly higher than for UHMWPE. In 1994, Hall et al. [58] reported dry friction factors of UHMWPE in Charnley THRs of 0.11-0.16, where as in 2006, Scholes et al. [79] reported friction factors of roughly 0.8-1.0 for PU in a THR. During daily activities, a joint is always adequately lubricated, assuring that the lubrication film does not break down. However, after prolonged inactivity of the joint, it is possible that the fluid may be drawn through the joint space [36, 79], thus increasing the risk of direct contact between the articulating surfaces and hence possibly higher friction. This phenomena is often described as start-up friction. A 1993 study by Caravia et al. [88] investigated start-up friction of different thin PU layers (pin-on-disk experiments) by applying a static load for a certain amount of time before commencing sliding. This was performed either in a dry state or immersed in deionized water. It was found that start-up friction depended on indenter roughness, PU elastic modulus and especially on static loading. Maximal COFs for start-up varied between 0.6 and 1.16, approaching the dry friction values reported earlier. On the other hand, steady state COF were found to be
as low as 0.02. The authors concluded that even though start-up friction was found to be very high, once implanted into the body, a cushion form bearing would be lubricated with synovial fluid which contains boundary lubricants, whose presence could prevent direct contact of the articulating surfaces [36].

Jin et al. assessed wear (weight loss) and friction of thin PU layers sliding on stainless steel disks [94]. Different lubrication regimes and PU pin geometries were considered. The experiments showed start-up friction of as high as 0.2, while steady state friction varied between 0.003 and 0.035 depending on the geometry. In conclusion, the authors found that as long as a full fluid film is maintained, COFs and wear will be much lower than in UHMWPE. However, should the fluid film break down, then wear can be two orders of magnitudes higher than in UHMWPE [94]. More recently, Scholes et al. [79] have investigated the issue of start-up friction using a hip friction simulator. The joint was statically loaded for one to twenty minutes, before being subjected to a walking simulation. Friction factors for start-up varied between roughly 0.08 and 0.55 depending on the loading time. Such high values could not be tolerated for a longer period of time. However, it was found that once the joint started to move, friction factors reduced quickly to low steady state values within one cycle. The results highlighted that the joint functioned under full fluid film lubrication within less than half a cycle.

A study by Stewart et al. from 1997 [73] investigated friction in TKRs under adverse conditions. A higher than usual cyclic peak load of 2000N (1000-1600N corresponds to normal walking [102]), lower entraining velocities and reduced stroke length were applied and friction was measured using four different lubricants (deionized water, CMC, bovine serum and high-viscosity oil). Normal walking conditions were also tested. It was shown that friction factors during adverse conditions were significantly higher than in normal conditions (0.15 vs 0.02), and bovine serum generally resulted in slightly higher values than water. The study also reported relatively high start-up friction (higher than the transducer limit of 0.18). They found that articular surface damage to be dependent on the
initial lubricant regime. When EHL was present, no damage was found, while initial mixed lubrication resulted in surface damage under adverse conditions. The conclusion was that a compliant tibial inlay ought to be designed to operate under elastohydrodynamic fluid films.

Another concern is debonding of the soft compliant layer from its harder substrate. In wear studies on TKRs from 1995, Auger et al. found that a soft PU layer with an elastic modulus of 6MPa failed due to almost complete debonding of the layer from its substrate resulting in a lot of wear debris, while an inlay made from PU with an elastic modulus of 20MPa inlay was less prone to delamination [74]. Overall, it was found that debonding was the limiting factor for long-term survival of this design. A finite element simulation [86] has found that the most likely place of failure of a compliant implant will be at the interface of the soft layer and the substrate. Considering the fact that debonding can be a cause of failure, Burgess et al. [93], in 2008, investigated the interface strength of a soft and hard PCU (substrate) layer by performing peel tests. Different manufacturing techniques to bond the two materials were investigated. The materials investigated possessed very similar chemical structures, which allowed strong diffusion bonds to be formed. In fact, in some tests the specimens failed because of tearing rather then peeling, indicating that the strength of the bond between the layers was equivalent to or greater than the cohesive strength of the specimens. It was also found that soaking the specimens in 37°C Ringer solution did not weaken the bond strength. It could be shown that when the materials were moulded under optimal conditions, a sufficient interface strength can be achieved. Using these results, Jones et al. [77] have conducted TKR wear test simulations for up to five million cycles at conditions similar to those experienced in vivo under normal walking. It was shown that the lateral part of the tibial inlay demonstrated some separation of the two layers. The extent of the separation was dependent on the layer thickness. Applying excessive malalignment caused the inlay to be pushed out of place (the resulting forces were too high and overcame the snap-fit mechanism). This was believed to be due to impingement of the
femoral component against the lateral tibial component. In order to determine whether
the debonding and the dislocation of the tibial inlay are due to material characteristics or
design limitations (a design optimized for UHMWPE was used), a second different design
was tested for two million cycles. No debonding or dislocating due to misalignment was
observed in this second design. The authors concluded that with a correct design and
manufacture, compliant polymer TKRs are likely to perform well.

2.4.5 Aging Performance of PU

As presented earlier, most of the compliant polymers investigated for materials in TJRs are
PUs. There are three basic types of PUs which are identified by the type of soft segment
present:

1. Polyester urethane: incorporating an ester linkage

2. Polyether urethane (PEU): incorporating ether moieties

3. Polycarbonate urethane (PCU): incorporating carbonate linkages

The composition of PUs will be discussed in more detail in Section 2.5.1. Table 2.4 provides
an overview of some commercially available PUs.

There have been concerns described in literature regarding the biostability of certain
PUs, namely those based on polyester and polyether [90, 91]. Some of the main degradation
mechanisms observed in PUs are hydrolysis, environmental stress cracking (ESC), metal ion
oxidation (MIO) and calcification [92] and these degradation mechanism are now defined
[103]:

- *Hydrolysis* is a reaction of a substance with water. Polyester urethanes are especially
  prone to hydrolysis due to the hydrolytic instability of the ester groups and have been
  shown to degrade and become fragmented within months.

- *Environmental Stress Cracking (ESC)* is an example of an oxidative degradation that
Table 2.4: Overview of commercially available polyurethanes

<table>
<thead>
<tr>
<th>Name</th>
<th>Supplier</th>
<th>Introduced in</th>
<th>Basic Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Estane®</td>
<td>Lubrizol, Ohio</td>
<td>1955</td>
<td>Polyether, Polyester</td>
</tr>
<tr>
<td>Biomer®†</td>
<td>DuPont, Delaware</td>
<td>1972</td>
<td>Polyether</td>
</tr>
<tr>
<td>Pelletane™</td>
<td>Dow Chemical, Michigan</td>
<td>1977</td>
<td>Polyether</td>
</tr>
<tr>
<td>Tecoflex®</td>
<td>Lubrizol, Ohio</td>
<td>1983</td>
<td>Polyether</td>
</tr>
<tr>
<td>Tecothane™</td>
<td>Lubrizol, Ohio</td>
<td></td>
<td>Polyether</td>
</tr>
<tr>
<td>Elasthane™</td>
<td>DSM PTG, California</td>
<td></td>
<td>Polyether</td>
</tr>
<tr>
<td>Bionate®‡</td>
<td>DSM PTG, California</td>
<td></td>
<td>Polycarbonate</td>
</tr>
<tr>
<td>Chronoflex©</td>
<td>Polymedica, Massachusetts</td>
<td></td>
<td>Polycarbonate</td>
</tr>
<tr>
<td>Carbothane®</td>
<td>Lubrizol, Ohio</td>
<td></td>
<td>Polycarbonate</td>
</tr>
</tbody>
</table>

† Biomer® was formerly branded as Lycra
‡ Bionate® was formerly branded as Corethane®

degrades the average molecular weight of a polymer and therefore its mechanical properties. This phenomenon involves crazed crack (micro-fissure) formation and propagation. It is thought that ESC is due to a combination of mechanical stress (residual or external) and exposure to a chemical environment. It involves oxidation of the surface, usually explainable by a decreasing soft segment ether concentration, and residual stress. ESC seems to be related to the ether content since the resistance against it increases with decreasing ether content (therefore increasing hardness). Polyether urethane can be strongly affected by oxidative degradation. Polycarbonate urethane has been shown to be more resistant to ESC than polyether urethanes.

- **Metal Ion Oxidation (MIO)** is an oxidative degeneration catalyzed by metal ions, which are the corrosion product of metal components. Polymers effected by MIO typically show deep brittle cracks typical of a high rate of loading. Unlike ESC, MIO can also occur in the absence of residual stress. The process usually starts at the metal-polymer-interface where MIO may be greatest. Polyether urethane may undergo MIO,
while polycarbonate urethane has been shown to have excellent resistance to MIO [92].

- **Calcification** is the deposition of calcium containing apatite mineral which causes polymers to become brittle [104].

A biomaterial needs to provide certain mechanical and physical properties, and needs to be biocompatible in order to be satisfactory for a particular application. Williams defined biocompatibility as follows:

*Biocompatibility refers to the ability of a biomaterial to perform its desired function with respect to a medical therapy, without eliciting any undesirable local or systemic effects in the recipient or beneficiary of that therapy, but generating the most appropriate beneficial cellular or tissue response in that specific situation, and optimising the clinically relevant performance of that therapy* [67].

The biological response of PU is generally acceptable; however, there have been issues with initial expectation of long-term usage of PU-based devices due to degradation (for example in pacemaker lead encapsulation). One problem of studying PU degradation and improvement is the lack of standardized tests. Currently, the best way to test seems to be *in vivo* animal studies, since the most trusted data on biocompatibility is derived from an actual clinical application of the material [67].

Polyester urethanes were the first PUs used in medical applications, but were later replaced by polyether urethanes (PEU) because of hydrolysis affecting the polyester soft segments, making them unsuitable for long-term implantation. However, PEU has been shown to be prone to MIO and in some cases, such as pacemaker lead insulation, ESC [90, 91, 104–106].

In 1995, Stokes *et al.* [105] conducted early *in vitro* studies on the hydrolytic, ESC and MIO resistance of PCU (ChronoFlex). No sign of hydrolysis, ESC or MIO were reported at the time, although a PEU tested at the same time showed severe ESC. The resistance
against hydrolysis was speculated to be due to the low water permeability of PCU. Tanzi et al. (2005) developed an in vitro procedure to test the oxidative stability of PUs. One PEU, Pellethane, and three PCUs, Corethane, Bionate and Chronoflex, all with a shore hardness of 80A, were investigated. Thin sheets were strained to 100% and together with unstressed samples immersed in two different aging solutions (alkaline and acidic) for seven days at 50°C. The surface morphology of the specimens was analysed before and after the aging treatment using scanning electron microscopy (SEM). Tensile tests to fracture before and after the oxidation experiments were also carried out. In addition, the same tests were performed on tubular specimens cut from two commercial catheters produced from a PEU (Tecoflex) and a PCU (Carbothane). Overall, it was found that PEU showed more degradation in alkaline conditions whereas PCU was more affected by the acidic agent. However, PCU was generally more stable than PEU. The tests on catheters supported the results obtained from thin film experiments, showing that PCU is more stable than PEU.

Wiggins et al. (2004) compared the biostability of PEU and PCU by means of fourier transform infrared microscopy (FTIM microscopy) to assess the chemical degradation [91]. SEM was used to analyse the physical damage following an in vitro fatigue and creep experiment in CoCl₂/H₂O₂ solution that reproduces the oxidative component of an in vivo environment. The thin films were immersed in this solution and subjected to dynamic and static loading for up to 24 days. Moreover, the polymers were mechanically characterized using dynamic mechanical thermal analysis (DMTA) and simple tension. Four different PUs were investigated, among them a PEU (Elasthane 80A) and a PCU (Bionate 80A). The accelerated in vitro experiment revealed that PCU’s resistance against oxidative degradation is superior to that of PEU. Degradation of the polycarbonate soft segment was minimal while oxidative chain scission and cross linking of the polyether soft segments resulted in brittle surface layers with pits and dimples. However, it was found that PCU showed markedly less creep resistance and the ultimate strain to failure when loaded in tension was lower than of PEU.
In a 2004 study performed by Christenson et al. [90], the effect of the soft segment of PUs on the \textit{in vivo} biostability was investigated. PEU (Elasthane 80A) and PCU (Bionate 80A) films and tubes with similar hard-to-soft segment ratios were used. DMTA and uniaxial tension tests were conducted using the PU films. The PCU specimens were shown to have higher modulus and reduced ultimate elongation than PEU. This was attributed to the reduced flexibility of the polycarbonate soft segment. The surfaces of all of the PUs were characterized using various techniques. \textit{In vivo} rat studies with biaxially strained tube specimens were conducted. Strained specimens were implanted into young rats and explanted after 5 to 20 weeks to assess the surface degradation. From the short term \textit{in vivo} experiment it was concluded that both PUs can be assumed to be biocompatible. Surface analysis of the explanted specimens did not reveal any physical degradation. Since it has been previously shown that PEU may exhibit surface pitting and cracking, it was speculated that the lack of damage found in this study was due to the short implantation time and high soft segment content. Analysis of the infrared spectrum of PEU indicated soft segment oxidation, while the analysis of PCU revealed changes in the soft and hard segment chemistry. Generally, it was found that both PUs were prone to chain scission and cross-linking during these tests. Christenson \textit{et al.} concluded that the biodegradation mechanisms of PCU ought to be further investigated.

A year later, Khan \textit{et al.} reported that PCU had excellent resistance against common biodegradation mechanisms. The group performed a comparative biostability \textit{in vitro} study of two PEUs (Pelletehane and PHMO-PU) and two PCUs (Chronoflex and Corethane (currently branded as Bionate (see Table 2.4))). Various accelerated aging experiments were conducted for up to three years to investigate the resistance of the PUs against hydrolysis, ESC, MIO and mineralization. Additionally, the polymers were mechanically characterized in tension tests. These tensile tests showed that PCU has a lower failure strain and a higher soft segment glass transition temperature than PEU which is due to the decreased flexibility of the polycarbonate component of the PCU. From all the PUs investigated over a 3-year
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period, Corethane 80A and PHMO-PU showed the highest resistance against hydrolysis. It was also shown that Pellethane and PHMO-PU are vulnerable to ESC, while the two PCUs exhibited good resistance to ESC. The PCUs showed excellent resistance against MIO, but the two PEUs were prone to MIO. Overall, Corethane 80A was found to be the most environmentally stable of the PUs investigated and Pellethane the least stable.

Several investigators have conducted in vivo studies to assess the aging performance of PCU. In 2003, Jones et al. [75] performed a four year ovine THR study using a PU acetabular cup. After explantation, a full histological analysis of the synovial fluid, surrounding tissue and remote organs was carried out, as well as physical, mechanical, microscopic and spectroscopic examination of the acetabular cups. The polymer chemistry was shown to be stable over time and showed no signs of degradation. More importantly, the material was well tolerated by the animal. In the previously described ovine THR study from 2004 by Khan et al. [80] (see Section 2.4.2) no significant physical or chemical degradation of the PCU cup was observed, suggesting that the implant functioned well in the sheep. Resistance against biodegradation was reported by Khan et al. to be excellent. The authors concluded that there is no contra-indication against human trials, although human trials were not reported in the study. The ovine hip study from 2006 by Carbone et al. (Section 2.4.2) revealed that the aging performance of PCU was excellent for up to 48 months. There was some necrosis evident in the 6-month group, however, the authors did not elaborate on that observation.

In 2006 in Europe, a human clinical study was commenced with the aim to evaluate PCU as a weight bearing material for THR. In 2008, two studies were published that each analysed one acetabular PCU cup retrieval [107, 108]. Both cups investigated were produced by Active Implants Corp. (Memphis, Tennessee). In the design used, a PCU cup is clipped directly into the bone and then used in combination with a conventional hip stem. One study examined a cup that was implanted for 12 months before it was retrieved due to hip pain (the pain was later attributed to a spine pathology) [107] and the other
study examined a cup that was explanted after 10.5 months because the patient experienced pain and the cup could not be seen on CT scans (at retrieval, the cup was shown to be undamaged) [108]. Wear and surface analyses of the acetabular cup were performed in both studies as well as analyses of histological samples and analyses of the synovial fluid. Both studies found low wear rates that were consistent with laboratory findings and ovine hip studies. Minimal tissue reactivity and no signs of synovites were found. Wear rates were lower than those usually found in UHMWPE retrievals and PCU wear particles were larger and fewer than what is usually expected with UHMWPE acetabular cups implanted over the same time period. Some abrasive macroscopic back side wear was observed, believed to be due to micromotion between the cup and the bone. The authors point out that the THR could be easily revised because only minimal bone had been removed upon primary implantation. Overall, the findings supported the concept of using PCU in load bearing articulation surfaces in THR/TKR.

### 2.4.6 Application of PU in Medical Devices

PUs are one of the most important materials in cardiac and vascular surgery. PU is used in cardiac valves, vascular prostheses, pacemakers lead encapsulation, and even entire artificial hearts. Other applications include bandages, tapes, catheters, tubes, cannulae, endoprostheses, wound dressings and cosmetic breast implants [103].

Apart from many *in vivo* and *in vitro* studies showing the potential of compliant polymers in general and specifically PCU in TJRs, there are also a few commercial products on the market using PCU in similar applications. Zimmer GmbH (Winterthur, Switzerland) has been using PCU in their Dynesys® dynamic lumbar spine stabilization system for many years (see Figure 2.17(a)). Another more recent product is a THR by Active Implants (Memphis, Tennessee), called Tribofit®. The Tribofit® system consists of a femoral stem and a metal acetabular cup that holds a two-layer PCU (Bionate) buffer, with a hard substrate and a soft buffer layer, as seen in Figure 2.17(b). The same company has
announced the launch of a PCU menisci substitute for early knee conditions, NuSurface™. Another spine implant, Physio-L®, an artificial lumber disc from the company NexgenSpine (Whippany, New Jersey), is also on the market. Two examples of other spinal implants on the market are the Bryan® Cervical Disc by Medtronic (Minneapolis, Minnesota) which consists of a polyurethane nucleus surrounded by titanium end plates and a full PCU total disc replacement called CAdisc™ by Ranier (Cambridge, UK). Table 2.5 lists an overview of available PU products.

### 2.4.7 Special Considerations for the Use of PCU in a TKR

PCU has been the subject of numerous investigations, is being applied in a range of medical devices and has been shown to have the potential to be used in a TKR. However certain aspects need to be considered:

- It is important that the TKR is designed in such a way that full fluid film lubrication is promoted
Table 2.5: Overview of some PU applications

<table>
<thead>
<tr>
<th>Application</th>
<th>Product Examples</th>
<th>Manufacturer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cardiac Valves</td>
<td></td>
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† to be launched in 2009

- The Soft layer and hard substrate should be of similar chemistry in order to ensure strong bonding between the two
- Certain design criteria, such has conformity and layer thickness need to be addressed for optimal performance
- Because of the dramatically different mechanical properties of UHMWPE and PCUs, it is unlikely that using existing designs which were developed for UHMWPE would be successful if applied to PCU

In this section, it was shown that PCUs are the most promising compliant polymers for use in TKRs. Therefore the next section will present some basic theory about PUs in general and PCUs in particular.
2.5 Structure and Properties of Polycarbonate Urethane PCU

In this section, the basic structure of PU and properties of the different types of PU will be discussed.

2.5.1 Polyurethane Background

Thermoplastic elastomers (TPEs) are rubber-like materials that combine the characteristics of rubbers, such as fast recoverability and large elongation to more than 100% with the easy processibility and recyclability of thermoplastics [109]. Elastomers are often distinguished by their hardness. The hardness of elastomers are typically measured on the Shore A or Shore D scale, where the A scale is softer than the D scale. Figure 2.18 shows the shore hardness range of TPEs compared to thermoset rubbers and hard thermoplastics. It is clearly visible that TPEs bridge the two hardness scales [9].

![Figure 2.18: Shore hardness range of TPE, adapted from Harper [9]](image)

One type of TPE are thermoplastic polyurethanes (TPUs), which were the first commercially available TPEs [10]. TPU is the generic name of a family of synthetic copolymers that contain the urethane moiety in their chemical repeat structure [103]. TPUs are different from most polymers, such as PET, PTFE, PS or PE, which possess a fairly simple chemical structure synthesized from one or two monomers. TPUs on the other hand, possess a more complicated structure typically comprising of three monomers. By varying the contents of
these monomers, essentially a limitless number of materials with various mechanical characteristics may be obtained. Polyurethane (PU) is available in a variety of applications including foam, paint, and adhesives [103].

Today approximately 15% of all TPEs are TPUs [9]. Otto Bayer (today Bayer AG) was among the pioneers in PU development [10]. Bayer and co-workers first synthesized PU in 1937. During the 1940s, PU was already being produced on an industrial scale. Early PUs consisted of three different parts:

1. Polyester or Polyether Macrodiol
2. a chain extender such as water, a short chain diol or a diamine
3. a bulky diisocyanate, e.g. naphthalene-1,5-diisocyanate (NDI)

However, these early versions were not real TPUs since their melt temperature was higher than the decomposition temperature and they could therefore not be thermally processed and recycled like thermoplastics. Subsequently, great progress was made when NDI was replaced by diphenylmethane-4,4-diisocyanate or MDI. Today it is widely known that TPUs owe their unique properties to a domain structure which is achieved by a phase separated system of these multi-block polymers [10].

One block, the hard segment, is built by adding chain extender (e.g. 1,4 butanediol BD) to the MDI. The second block, the soft segment, consists of long flexible polyether,
polyester, or polycarbonate chains which interconnect with two hard segments [10]. A simple schematic of this structure is illustrated in see Figure 2.19.

At room temperature, the low melting soft segments are incompatible with the polar high melting hard segments and this leads to a microphase separation. Part of what drives this separation is the crystallisation of hard segments. When heated above the melting temperature of the hard segment, the polymer forms a homogenous viscous melt that can be processed just as any thermoplastic (e.g. injection moulding, extrusion etc). Subsequent cooling leads again to phase separation [10].

Normally, soft segments form an elastomeric matrix accounting for the reversibly elastic properties and hard segments act as physical crosslinks and reinforcing fillers. Unlike chemical crosslinks in elastomers, physical crosslinks in TPU can be overcome by heat or solvation, giving TPUs the aforementioned good processibility of thermoplastics [10].

The morphology of multiphase systems, such as TPUs, is an important determinant of the final mechanical properties of a product. By varying the morphology, the desired properties can be obtained. Therefore, a deep understanding of the morphology is crucial for understanding the relationship between structure and mechanical properties. The urethane block polymers structure is complicated by crystallisation, inter-phase mixing, hydrogen bonding in both phases [10].

In theory, the phase separation occurs due to the thermodynamic incompatibility of the phases (positive mixing enthalpy). As the number of blocks in a copolymer molecule of given length increases, the phase separation becomes increasingly more difficult. Conversely, increasing the molecular weight at fixed copolymer composition and number of blocks per molecule would favour phase separation. In general, it is said that the phase separation is more complete when one component is crystallisable. Soft segments are usually in the amorphous state and only crystallise at very low hard segment content or prolonged cooling. Phase separation is often incomplete where some hard segments are isolated in the soft segment matrix (see Figure 2.20(b)) [11]. Depending on the hard segment content, one
CHAPTER 2. LITERATURE REVIEW

(a) Low hard segment content in a soft segment matrix

(b) High hard segment content and isolated hard segments in soft segment matrix

Figure 2.20: Hard and soft segment arrangement in TPUs, adapted from Qi et al.[11]

observes hard domains ranging from isolated domains (see Figure 2.20(a)) to interconnected domains as can be seen in Figure 2.20(b) [11].

The low temperature properties are governed by the broadness and location of the glass transition range of the soft segment. The range starts with the first melting of the amorphous soft segments and ends with soft segments being completely molten. The broadness of the range depends on the hard segment content and the separation of hard and soft segment. In general, the higher the hard segment content, the broader the range and the higher the glass transition temperature. Such a polymer with high hard segment content may be expected to be more brittle at lower temperature. The shifting of the glass transition temperature might be explained by more hard segments being “dissolved in the soft phase, leading to a concentration gradient of hard segments close to the phase separation interface. This phenomenon has been attributed to irregular phase interface structures. Figure 2.21 (left) shows a possible schematic of such a structure in which the movement of fractions of the soft segments is greatly restrained. These fractions need elevated temperatures in order
to become flexible. The low temperature flexibility can be improved by using soft segments which are less compatible with hard segments, which brings the start of the glass transition temperature well below room temperature and narrows the range. It has been reported that annealing also increases the incompatibility and therefore the phase separation [105]. During annealing, the structure is rearranged into a thermodynamically more favourable arrangement, shown schematically in Figure 2.21 (right). Moreover, annealing has been shown to increase the repeatability of the material properties [10]. In addition, research has shown that, if properly performed, annealing can improve the resistance to ESC, since it reduces residual stress in the specimen [104, 110].

Polycarbonate urethane (PCU) is one type of TPU and in this work two different PCUs, known as Bionate® 55D and 80A (The Polymer Technology Group, California), with the following hard and soft segment contents were investigated (hereafter referred to as PCU55D and PCU80A):

- Bionate® 55D: 55% Soft Segments (Polycarbonate) and 45% Hard Segments (MDI, BD)
- Bionate® 80A: 65% Soft Segments (Polycarbonate) and 35% Hard Segments (MDI, BD)
PuS have been employed in medical applications since 1967 and the processibility and excellent mechanical behaviour make PuS an attractive candidate for implant materials. By altering the chemical structure, Pu can be tailor-made for many desired applications. Because the mechanical properties of PCU are so dependant on structure and thermomechanical history, it is difficult to fully characterise them in every loading scenario. Finite element analysis may be used to simulate a greater range of loading scenarios than may be practically performed. Some of the background of FEA will now be introduced.

## 2.6 Finite Element Analysis FEA - Background

Finite Element Analysis (FEA) is the most widely employed procedure to solve complicated mechanical problems, when it is too difficult or time consuming to state the algebraic equations (see equation 2.3) necessary to solve the problem for the entire domain. It is based on the discretisation of a body into a finite number of elements, a so-called mesh. The discretisation is performed in order to simplify a complicated problem into small manageable parts and hence, achieve a converged solution which is in equilibrium. At first, the algebraic equations are formulated for each single element and at the end all the elements equations are put together to formulate the global system matrix:

\[
K^E\{u_E\} = \{F^E\} \rightarrow K\{u\} = \{F\},
\]  

(2.3)

where \( K \) is the stiffness matrix (elasticity tensor), which is a function of the unknown displacement vector, \( u \), and \( F \) is the load vector.

In the following section, the basic mathematics of continuum mechanics necessary to solve engineering problems using FEA will be presented.
2.6.1 Continuum Mechanics

The following is a short summary of some basic continuum mechanics, which is described in more detail elsewhere [12].

Continuum mechanics is a method used to explain physical phenomena without knowing the full details of the complex internal structure of a body and is often called a macroscopic approach. In a continuum, the very large number of particles of a body are substituted by a few quantities, which represent averages over dimensions still small enough to reflect some microstructural effects. A continuum is assumed to have a continuous or piecewise distribution of matter or particles in space and time, where particles are considered to be an accumulation of a large number of molecules. There are three basic aspects of continuum mechanics: 1. the study of motion and deformation, also called kinematics, 2. the study of stress in a continuum and 3. mathematical descriptions of fundamental laws of physics governing the motion of a continuum (balance principles).

Kinematics

A continuum body can be described in different regions at different instances of time. As a body moves, it passes through those different regions, called configurations of the body. At \( t = 0 \) the body is in its fixed, initial, undeformed reference configuration and at \( t > 0 \) it is in its current or deformed configuration. The position of a particle, \( P \), in the reference configuration is denoted by \( X_I \) with the material or referential coordinates \( I = 1, 2, 3 \), while in the current configuration it is denoted by \( x_i \) with spatial or current coordinates \( i = 1, 2, 3 \).

There are two ways to describe the motion of a particle, either with respect to its material coordinates \( X_I \) and time \( t \) or its spatial coordinates \( x_i \) and time \( t \). The former is called the material or referential description, often called Lagrangian description, and the focus is on the particle while it moves through space and time. The latter description is called Eulerian or spatial description and attention is paid to a point in space and the changes in time at
this point are being described. In solid mechanics, both descriptions are used, however, the
Lagrangian description is often preferred. The Eulerian description is most often used in
fluid mechanics.

The displacement, $U(X,t)$, of a particle of a body in the Lagrangian description can be
described as the difference between its position in the deformed configuration, $x_i$, at time $t$
and its initial position, $X_I$, and is defined as (see Figure 2.22)

$$U(X,t) = x(X,t) - X.$$  \hspace{1cm} (2.4)

It relates the initial position to its position in the deformed configuration at time $t$. In
the Eulerian description, the displacement, $u(x,t)$, is a function of the current position and
time and is defined as

$$u(x,t) = x - X(x,t).$$  \hspace{1cm} (2.5)

The two descriptions for the displacement are identical in value

$$U(X,t) = u(x,t).$$  \hspace{1cm} (2.6)

Two particles that are close to each other are identified by their positions $X$ and $X+dX$,
where $X$ is a position vector and $dX$ the distance between the two particles. After deforming
the body, the distance between the two changes to $dx$. Using a linear mapping tensor, the
deformation gradient, $F$, the change occurring from the reference frame to the current frame
can be described using the following relation:

$$dx = FdX$$  \hspace{1cm} (2.7)
where the deformation gradient is defined as follows:

\[ F = \frac{\partial x}{\partial X} = \frac{\partial}{\partial X} (X + u) = I + \frac{\partial u}{\partial X} \quad (2.8) \]

and using index notation:

\[ F_{ij} = \frac{\partial x_i}{\partial X_j} = \frac{\partial}{\partial X_j} (X_i + u_i) = \delta_{ij} + \frac{\partial u_i}{\partial X_j}. \quad (2.9) \]

The deformation gradient is a very important quantity in nonlinear continuum mechanics and is a second order tensor with nine components. It is often called a two-point tensor, because it links points in two different configurations. The deformation gradient can be decomposed into pure stretch, \( \mathbf{U} \) or \( \mathbf{v} \), and pure rotation, \( \mathbf{R} \), using polar decomposition:

\[ \mathbf{F} = \mathbf{R} \mathbf{U} = \mathbf{v} \mathbf{R}. \quad (2.10) \]
If a body undergoes rigid motion and therefore no deformation is occurring, then the de-
formation gradient is equal to the identity tensor, $I$:

$$ F = I . $$

(2.11)

Another important entity in continuum mechanics is the determinant of the deformation
gradient, the Jacobian determinant, $J$:

$$ J = \det(F) $$

(2.12)

which is a measure of volume change. Physically, the volume change has to be positive,
therefore $J > 0$ must be satisfied at all times. $J$ becomes 1 when there is no motion at all,
or when the motion or deformation is volume-preserving (isochoric).

The velocity gradient tensor, $L$, is another important nonlinear continuum mechanics
measure. It is defined as the gradient of the velocity, $v$, and can be decomposed into the
rate of deformation tensor, $D$, and the rate of rotation tensor, $W$:

$$ L = \nabla(v) = \frac{\partial v}{\partial x} = D + W . $$

(2.13)

The velocity gradient tensor is, for example, used to calculate the time derivative of the
deformation gradient:

$$ \dot{F} = LF $$

(2.14)

Apart from describing the changes of material elements using displacement, strain quantities
can also be used. Strains, unlike displacements, cannot be directly measured and are merely
based on a concept introduced to simplify analyses. A short summary of the more common
material and spatial strain tensors now follows. Very common material strain entities are
the right Cauchy-Green tensor and the Green-Lagrange strain tensor, $C$ and $E$, respectively.
Both are symmetric and are defined as follows:

\[ C = F^T F \]  \hspace{1cm} (2.15)

\[ E = \frac{1}{2} (F^T F - I) = \frac{1}{2} (C - I) , \]  \hspace{1cm} (2.16)

where \( F^T \) is the transpose of the deformation gradient. Strain quantities associated with the current configuration, so-called spatial strain tensors, are the left Cauchy-Green tensor (Finger deformation tensor), \( B \), and the Euler-Almansi strain tensor, \( e \), which both are symmetric and defined as follows:

\[ B = F F^T \]  \hspace{1cm} (2.17)

\[ e = \frac{1}{2} (I - F^{-T} F^{-1}) . \]  \hspace{1cm} (2.18)

**Concept of Stress**

A consequence of the interaction (motion and deformation) between a material and a neighbouring material within a body is stress, which is defined as force per unit area. In nonlinear continuum mechanics, many different stress measures are used. Some important second-order stress tensors will now be described [12].

Depending on whether stress is described in the Lagrangian (material) description, the Eulerian (spatial) description or a combination of both, different stress definitions are used. A frequently used stress measure is the symmetric Cauchy stress tensor, \( \sigma \), which is often called true stress. It takes into account the changing contact area where pressure is applied to and is defined entirely in the Eulerian description (current configuration). Stress outputs in ABAQUS (Version 6.8-1, Dassault Systèmes Simulia Corp., Providence, Rhode Island) [13], which was used in this thesis, are Cauchy stress values. Another widely used second-order stress tensor is the first Piola-Kirchhoff stress tensor, \( P \). It asymmetric and can be
derived from the Cauchy stress tensor:

\[ P = J\sigma F^{-T}. \] (2.19)

This stress tensor value is a so-called two-point tensor, because it is calculated using forces acting in the current (Eulerian) configuration and the initial contact area defined in the material (Lagrangian) configuration. It is commonly known as the nominal stress tensor. Another important stress tensor in the Eulerian description is the symmetric Kirchhoff stress tensor, \( \tau \), defined as:

\[ \tau = J\sigma. \] (2.20)

A last second-order stress tensor that is sometimes used, is the symmetric second Piola-Kirchhoff stress tensor, \( S \) which has no real physical meaning. It can be derived from the Cauchy stress tensor using the following relation:

\[ S = JF^{-1}\sigma F^{-T}. \] (2.21)

In the case of small strains and small rotation it may be assumed that all the stress values are approximately equal (\( \sigma \approx P \approx \tau \approx S \)). Figure 2.23 provides a schematic of the stress tensors described here, and how they relate to each other.

**Governing Equations of FEA**

In order to achieve a converging solution of a structural problem, several fundamental balance principles are solved by the FEA program. These principles include conservation of mass, momentum balance and balance of energy. A summary of these governing equations now follows [12].

The mass of a body in non-relativistic physics is a constant value and neither increases nor decreases. Hence, the mass of a particle in the current configuration is the same as
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Figure 2.23: Different stress tensors and how they are related to each other in the reference configuration. The conservation of mass is described with the following general equation:

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{v}) = 0 \quad (2.22)
\]

where \( \rho \) is the density and \( \mathbf{v} \) the velocity.

In general mechanics, forces and moments need to be in equilibrium as defined by the first and second Newton’s principles of motion. In the context of continuum mechanics, the momentum balance principles, the linear momentum and the angular momentum, are the equivalent of these two Newton’s laws. The linear momentum is described as follows:

\[
\text{div}(\boldsymbol{\sigma}) + \mathbf{b} = \rho \mathbf{\dot{v}} \quad (2.23)
\]

and the angular momentum as:

\[
\boldsymbol{\sigma} = \boldsymbol{\sigma}^T, \quad (2.24)
\]

where \( \boldsymbol{\sigma} \) is the Cauchy stress, \( \mathbf{b} \) the body forces (i.e. gravity) and \( \mathbf{\dot{v}} \) the acceleration.

From the balance of linear momentum (equation 2.23), follows the balance of mechanical energy, which states that the sum of the rate of kinetic energy and the rate of internal
mechanical work (stress power) is equal to the rate of external mechanical work (external mechanical power):

\[
\frac{D}{Dt} \int_{\Omega} \frac{1}{2} \rho v^2 \, dv + \int_{\Omega} \boldsymbol{\sigma} : \mathbf{D} \, dv = \int_{\partial \Omega} t \cdot \mathbf{v} \, ds + \int_{\Omega} \mathbf{b} \cdot \mathbf{v} \, ds
\]  

(2.25)

where \( \boldsymbol{\sigma} \) the true stress, \( \mathbf{D} \) the rate of deformation tensor, \( t \) the surface traction and \( \mathbf{b} \) the body force (i.e. gravity).

Many efficient finite element formulations make use of the principle of virtual work. It is based on applying virtual (not real), arbitrary, infinitesimal displacements (perturbations), \( \partial \mathbf{u} \), to a body away from the current configuration. The finite element method requires the above described balance laws to be formulated in the form of variational principles. The virtual work is based on variational forms of the balance principles. In the principle of virtual work, the virtual internal work, \( \partial W_{int} \), is set equal to the external virtual work, \( \partial W_{ext} \).

\[
\int_{\Omega} \boldsymbol{\sigma} : \partial \mathbf{e} \, dv = \int_{\partial \Omega} t \cdot \partial \mathbf{u} \, ds + \int_{\Omega} \mathbf{b} \cdot \partial \mathbf{u} \, ds
\]  

(2.26)

The principle of virtual work is applicable for any kind of material and it is the simplest variational principle and it states:

The virtual stress work \( \sigma : \partial \mathbf{e} \) at fixed \( \sigma \) is equal to the work done by the body force, \( \mathbf{b} \), and the surface traction, \( t \), per unit current surface along \( \partial \mathbf{u} \) removed from the current configuration. [12].

All of these governing equations are used to assemble the global system matrix, which is then solved:

\[
K \{ u \} = \{ F \}
\]  

(2.27)
In this section the basic mathematical equations and concepts using in continuum mechanics and FEA were discussed. These are necessary to use FEA to model the deformation behaviour of materials. In the next section these, concepts will be applied to formulate constitutive equations to model the deformation behaviour of elastomers.

2.7 Constitutive Modeling of Elastomers

The fundamental concepts described in Section 2.6 are indispensable to characterize kinematics, stresses and balance principles. They do not, however, reveal anything about the material itself; they cannot be used to distinguish materials. Distinguishing materials is achieved by formulating so-called constitutive laws which are mathematical equations used to determine the state of stress at any point \( \mathbf{x} \) of a continuum body at time \( t \), approximating the physical behaviour of a material. There are two basic approaches in modeling mechanical behaviour: a phenomenological approach, where the material is modeled as a continuum without taking the underlying microscopic structure of the material and its relation to the deformation into account, and a physically based approach where the constitutive law is related to the microscopic structure of the material [12].

The aim of this section is to briefly explain some of the mechanical behaviours that are typical for elastomers such as those investigated in this thesis and to discuss common elastomer modeling approaches.

2.7.1 Terminology of Elastomer Deformation Behaviour

Elastomers can be strained for several hundred percent and may exhibit time-dependent behaviour, hysteresis and softening under cyclic loading.
Large Strain Behaviour - Hyperelasticity

A more complete description of hyperelasticity has been presented by Holzapfel and will be summarised here for completeness [12].

The nonlinear, large deformation behaviour of elastomers is usually called hyperelasticity. A hyperelastic material assumes the existence of a Helmholtz free-energy function, $\Psi$, which is, for homogeneous materials, a function of the deformation gradient, $F$. Helmholtz free-energy for homogeneous materials is often called strain energy function or just strain energy. This describes the strain energy stored in a material per unit of reference (initial) volume. It is assumed that $\Psi = 0$ in the undeformed, reference configuration. The energy function can also be expressed in terms of the right Cauchy-Green tensor, $C$, and the Green-Lagrange strain tensor, $E$. The three formulations are equal:

$$\Psi(F) = \Psi(C) = \Psi(E).$$  \hspace{1cm} (2.28)

Knowing the energy function, the stress can be calculated by taking the derivative of the energy function with respect to certain strain quantities. Formulations for the true stress, $\sigma$, and second Piola Kirchhoff stress, $S$, are described in Equations 2.29 and 2.30, respectively.

$$\sigma = J^{-1}F \frac{\partial \Psi(C)}{\partial C} F^T$$  \hspace{1cm} (2.29)

$$S = 2 \frac{\partial \Psi(C)}{\partial C} = \frac{\partial \Psi(E)}{\partial E}$$  \hspace{1cm} (2.30)

Rubbers are commonly modeled as isotropic materials, where it is assumed that the material response in stress-strain experiments is the same in all directions. When isotropy is assumed, the strain energy can be expressed as a function of the three invariants of either the right or left Cauchy-Green ($C$ and $B$) tensors

$$\Psi = \Psi[I_1(C), I_2(C), I_3(C)] = \Psi[I_1(B), I_2(B), I_3(B)],$$  \hspace{1cm} (2.31)
hence, the Cauchy stress and second Piola-Kirchhoff stress can also be stated as a function of invariants:

\[
\sigma = 2J^{-1} \left( I_3 \frac{\partial \Psi}{\partial I_3} I + \left( \frac{\partial \Psi}{\partial I_1} + I_1 \frac{\partial \Psi}{\partial I_2} \right) B - \frac{\partial \Psi}{\partial I_2} B^2 \right) \quad (2.32)
\]

\[
S = 2 \left( \left( \frac{\partial \Psi}{\partial I_1} + I_1 \frac{\partial \Psi}{\partial I_2} \right) I - \frac{\partial \Psi}{\partial I_2} C + I_3 \frac{\partial \Psi}{\partial I_3} C^{-1} \right) \quad (2.33)
\]

If the strain energy function is an invariant then the strain energy may also be described as a function of the principal stretches \( \lambda_a \) (\( a = 1, 2, 3 \))

\[
\Psi = \Psi(F) = \Psi(\lambda_1, \lambda_2, \lambda_3) . \quad (2.34)
\]

The principal Cauchy stresses, \( \sigma_a \), and the principal second Piola-Kirchhoff stresses, \( S_a \), are then defined as follows

\[
\sigma_a = J^{-1} \lambda_a \frac{\partial \Psi}{\partial \lambda_a} , \quad a = 1, 2, 3 \quad (2.35)
\]

\[
S_a = \frac{1}{\lambda_a} \frac{\partial \Psi}{\partial \lambda_a} , \quad a = 1, 2, 3 \quad (2.36)
\]

where

\[
J = \lambda_1 \lambda_2 \lambda_3 . \quad (2.37)
\]

Many polymers are incompressible materials that can undergo significant strain without noticeable volume change. In order to account for incompressibility of isotropic materials a modified strain energy function is used:

\[
\Psi = \Psi(I_1(C), I_2(C)) - \frac{1}{2} p(I_3 - 1) = \Psi(I_1(B), I_2(B)) - \frac{1}{2} p(I_3 - 1) . \quad (2.38)
\]

where \( p \) is the hydrostatic pressure. Differentiation of equation 2.38 and mathematical reforming yields the relations

\[
\sigma = -pI + 2 \frac{\partial \Psi}{\partial I_1} B - 2 \frac{\partial \Psi}{\partial I_2} B^{-1} \quad (2.39)
\]
and

\[ \mathbf{S} = -p \mathbf{C}^{-1} + 2 \left( \frac{\partial \Psi}{\partial I_1} + I_1 \frac{\partial \Psi}{\partial \mathbf{I}_1} \right) \mathbf{I} - 2 \frac{\partial \Psi}{\partial I_2} \mathbf{C} \]  

(2.40)

for Cauchy stress and second Piola Kirchhoff stress as a function of the first and second invariant, respectively. For incompressible materials, \( I_3 = 1 \).

Analogous to equations 2.34 and 2.35, the principal stress of incompressible, isotropic material can be defined as a function of principle stretches:

\[ \sigma_a = -p + \lambda_a \frac{\partial \Psi}{\partial \lambda_a}, \quad a = 1, 2, 3 \]  

(2.41)

\[ S_a = \frac{1}{\lambda_a^2} p + \frac{1}{\lambda_a} \frac{\partial \Psi}{\partial \lambda_a}, \quad a = 1, 2, 3 \]  

(2.42)

where

\[ \lambda_1 \lambda_2 \lambda_3 = 1 \]  

(2.43)

In the case of compressible and nearly incompressible isotropic materials, it is often helpful to decompose the strain energy into the volumetric (or dilational or volume-changing) and the isochoric (or distortional or volume-preserving) elastic response. For the modified deformation gradient, the modified left and right Cauchy-Green tensor we obtain:

\[ \bar{\mathbf{F}} = J^{-\frac{1}{2}} \mathbf{F} \]  

(2.44)

\[ \bar{\mathbf{B}} = J^{-\frac{2}{3}} \mathbf{B} \]  

(2.45)

\[ \bar{\mathbf{C}} = J^{-\frac{4}{3}} \mathbf{C} \]  

(2.46)

\( \bar{\mathbf{B}} \) and \( \bar{\mathbf{F}} \) are associated with the isochoric deformation of the body. This separation is helpful in FEA to avoid numerical difficulties (see Section 3.2.1) in nearly incompressible materials and is also often used in elastoplasticity. The decomposition of the strain energy
yields the following relation:

$$\Psi(B) = \Psi_{\text{iso}}(\bar{B}) + \Psi_{\text{vol}}(J).$$

(2.47)

In the same fashion, the Cauchy and second Piola-Kirchhoff stress tensors can be decoupled into an isochoric and a volumetric part:

$$\sigma = 2J^{-1}B \frac{\partial \Psi(B)}{\partial B} = \sigma_{\text{iso}} + \sigma_{\text{vol}}$$

(2.48)

$$S = 2\frac{\partial \Psi(C)}{\partial C} = S_{\text{iso}} + S_{\text{vol}}.$$  

(2.49)

Finally the strain energy for compressible or nearly incompressible isotropic materials can be formulated in terms of invariants:

$$\Psi = \Psi_{\text{iso}}[\bar{I}_1(\bar{C}), \bar{I}_2(\bar{C})] + \Psi_{\text{vol}}(J) = \Psi_{\text{iso}}[\bar{I}_1(\bar{B}), \bar{I}_2(\bar{B})] + \Psi_{\text{vol}}(J).$$

(2.50)

where the modified invariants are defined as follows:

$$\bar{I}_1 = tr(\bar{C})$$

(2.51)

$$\bar{I}_2 = \frac{1}{2} \left( (tr\bar{C})^2 - (tr\bar{C}^2) \right) = \frac{1}{2} \left( (tr\bar{B})^2 - (tr\bar{B}^2) \right)$$

(2.52)

$$\bar{I}_3 = det\bar{C} = det\bar{B} = 1.$$  

(2.53)

Up to now the general forms of the strain energy function of hyperelastic materials have been discussed. A short list of some specific forms of strain energy functions that have been developed over time for isotropic, incompressible and compressible materials is now described. Table 2.6 gives an overview of typical strain energy functions for incompressible materials. More detailed descriptions can be found in [12] and literature specific to the individual models. In the case of compressible or nearly incompressible materials,
Table 2.6: Some strain energy functions for incompressible materials

<table>
<thead>
<tr>
<th>$\Psi$</th>
<th>Equation</th>
<th>Note</th>
<th>Function of</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ogden</td>
<td>$\sum_{p=1}^{n} \frac{\mu_p}{\alpha_p} (\lambda_1^{\alpha_p} + \lambda_2^{\alpha_p} + \lambda_3^{\alpha_p} - 3)$</td>
<td>$\mu$: shear modulus</td>
<td>Principal Stretches</td>
<td>1</td>
</tr>
<tr>
<td>Mooney-Rivlin</td>
<td>$\frac{\mu_1}{2} (I_1 - 3) + \frac{\mu_2}{2} (I_2 - 3)$</td>
<td>$\mu = \mu_1 - \mu_2$</td>
<td>Invariants</td>
<td>1</td>
</tr>
<tr>
<td>Neo-Hookean</td>
<td>$\frac{\mu}{2} (I_1 - 3)$</td>
<td>$\mu = \mu_1$</td>
<td>Invariant</td>
<td>1</td>
</tr>
<tr>
<td>Yeoh</td>
<td>$c_1(I_1 - 3) + c_2(I_1 - 3)^2 + c_3(I_1 - 3)^3$</td>
<td>$\mu = 2c_1 + 4c_2(I_1 - 3) + 6c_3(I_1 - 3)^2$</td>
<td>Invariant</td>
<td>1</td>
</tr>
<tr>
<td>Arruda-Boyce</td>
<td>$\mu \left( \frac{(I_1 - 3)}{2} + \frac{(I_1^2 - 9)}{20n} + \frac{(I_1^3 - 27)}{1000n^2} + \ldots \right)$</td>
<td>n: number segments in chain; $\sqrt[3]{I_1} = \sqrt[3]{3\lambda_{\text{chain}}}$; $\lambda_{\text{chain}}$: stretch of a chain</td>
<td>Invariant</td>
<td>2</td>
</tr>
</tbody>
</table>

1: Phenomenological; 2: Statistical (physical)

the hitherto described decoupling is also applied to the specific strain energy functions in Table 2.6. Hence, strain energies that are a function of invariants, such as the Yeoh model are described as:

$$\Psi(\bar{I}_1, J) = c_1(\bar{I}_1 - 3) + c_2(\bar{I}_1 - 3)^2 + c_3(\bar{I}_1 - 3)^3 + \Psi_{\text{vol}}(J) .$$  \hfill (2.54)

Other models are formulated in the same manner. It is important to know that the exact formulation of these strain energy function slightly vary depending on the reference used.

**Hysteresis**

The nonlinear elasticity described above assumes that the behaviour of a material upon unloading is the same as during loading. However, this is usually not the case. The unloading stress-strain curve is sometimes significantly different to the loading curve. The
complete loading-unloading curve forms a “loop”; the stress upon unloading is lower than upon loading at the same strain level.

**Time Dependency - Viscoelasticity**

Apart from nonlinear elasticity, the mechanical behaviour of elastomers is also known to be rate-dependent and time-dependent. Examples of time-dependency are the mechanical response under a constant load, creep, the delayed strain recovery upon unloading and the stress relaxation under a constant deformation. The mechanical response of a viscoelastic solid depends on the history of its deformation. A more complete description of viscoelasticity has been presented by Wineman [111] and in the Abaqus 6.8 Manual [13] and will be summarized here for completeness.

There are basically two different types of viscoelastic behaviour: linear and nonlinear viscoelasticity. The former applies to small deformations and the latter applies in finite larger deformations. Linear viscoelasticity is briefly discussed first.

The term creep describes the deformation behaviour of a viscoelastic material subject to an instantaneously increased stress that is then fixed. Typically, upon application of stress, the strain response consists of an immediate increase in strain (elastic response) which is then followed by a continuous straining until it asymptotically approaches a certain strain value at $t \to \infty$. The fact that the strain reaches a finite value indicates solid behaviour. Creep is commonly described with the creep function, $J(t, \sigma_0)$, that includes the instantaneous response, $J(0, \sigma_0)$, and equilibrium response, $J(\infty, \sigma_0)$, for $t = 0$ and $t \to \infty$, respectively. Stress relaxation is the behaviour of a viscoelastic material subject to an instantaneously increased strain which is then fixed. Typically, upon strain application, the stress response consists of an instantaneous increase in stress (elastic response) which is then followed by a continuous stress relaxation until it asymptotically approaches a certain stress value at $t \to \infty$. The fact that the stress reaches a finite value indicates solid behaviour. Stress relaxation is commonly described with the stress relaxation function, $G(t, \epsilon_0)$, that
incorporates the instantaneous response, $G(0, \epsilon_0)$, and equilibrium response, $G(\infty, \epsilon_0)$, for $t = 0$ and $t \rightarrow \infty$, respectively. The stress relaxation function is a time-dependent elastic modulus and hence $E(t, \epsilon_0)$ will hereafter be used. Both the stress relaxation function and the creep function are material properties.

Linearity in viscoelasticity implies that if the strain is scaled by a constant, then the corresponding stress is also scaled by the same factor. The same is true for the case when stress is scaled by a factor, and the resulting strain is also scaled by this factor. Another assumption of linearity is that if two strain histories are superimposed, the corresponding stresses are also superimposed and vice versa. Linearity in this case does not refer to the shape of any material response behaviour when plotted in a stress vs. strain graph.

Viscoelasticity in Abaqus can be defined in the time domain and frequency domain; however, the latter will not be considered in this section [13]. The stress is formulated with the following basic hereditary integral formulation

$$\sigma(t) = \int_0^t 2G(\tau - \tau') \dot{e} \, dt' + I \int_0^t K(\tau - \tau') \dot{\phi} \, dt'$$ (2.55)

where $e$ and $\phi$ are the mechanical deviatoric and volumetric strains, respectively. $K$ is the bulk modulus and $G$ the shear modulus, which are a function of the reduced time, $\tau$. The two relaxation functions $G(t)$ and $K(t)$ are defined with a so-called Prony series, which is a series of exponential functions:

$$K(t) = K_\infty + \sum_{i=1}^{n_K} K_i e^{-\tau/\tau^K_i}$$ (2.56)

$$G(t) = G_\infty + \sum_{i=1}^{n_G} G_i e^{-\tau/\tau^G_i}.$$ (2.57)

Here $K_\infty$ and $G_\infty$ are the long-term bulk and shear moduli and $\tau^K_i$ and $\tau^G_i$ the relaxation times which Abaqus assumes to be equal [13]. $n_K$ and $n_G$, the number of terms, on the
other hand, are not necessarily equal. $n_K$ is often taken to be 0. Equations 2.56 and 2.57 can be rewritten in the following manner:

$$K(t) = K_0 \left( \alpha_{\infty}^K + \sum_{i=1}^{n_K} \alpha_i^K e^{-\tau_i^K/\tau_i^K} \right)$$

(2.58)

$$G(t) = G_0 \left( \alpha_{\infty}^G + \sum_{i=1}^{n_G} \alpha_i^G e^{-\tau_i^G/\tau_i^G} \right)$$

(2.59)

where $G_0$ and $K_0$ are the instantaneous shear and bulk moduli, respectively, $\alpha_i = G_i/G_0$ is the relative moduli and $\alpha_{\infty} = G_{\infty}/G_0$ is the long-term relative modulus. The time constants, the relative moduli and the long-term relative modulus are the material properties defined in the Abaqus viscoelastic material property [13]. Either creep or relaxation test data can be used to determine these constants.

In nonlinear viscoelasticity the material behaviour becomes stress and strain dependent and scaling and superimposition are no longer applicable. The theory of nonlinear viscoelasticity makes use of the continuum mechanics described in Section 2.6.1 with the addition of time-dependency. A very detailed derivation of nonlinear viscoelasticity has been presented elsewhere [111]. Abaqus uses a time domain generalization of the hyperelastic constitutive models, where it assumes that the instantaneous response follows from the hyperelastic model [13]. The relaxation moduli defined in equations 2.58 and 2.59 are also used here. The stress formulation, which will not be described here, is decoupled into a deviatoric and a hydrostatic part. This concept has also been described in Section 2.7.1 for hyperelastic constitutive equations and is described in more detail elsewhere [13].

**Softening - The Mullins Effect**

In this section, the stress softening that is observed in some elastomers will be presented based on a review of the Mullins Effect by Diani et al. [112] and the Abaqus Manual [13].
Figure 2.24: Example of a typical tension data set exhibiting the Mullins effect, adapted from the Abaqus manual [13]. In this example, a specimen is first loaded and unloaded for several cycles, before the strain is increased and the specimen loaded and unloaded again before the strain is increased for a third time and the specimen is again loaded and unloaded for several cycles. It is clear for every strain level shown in different colours, that the first loading cycle is different to subsequent cycles.

Stress softening is a phenomenon observed during cyclic loading of elastomers. It describes the phenomenon where the stress required to reload, after a specimen has been previously loaded and unloaded, is less than the stress that was necessary during the previous loading for stretches up to the maximum achieved in the previous loading. Stress softening is commonly referred to as the Mullins Effect due to the fact that Mullins was the first person to extensively report the phenomenon in the 1960s [113]. Figure 2.24 shows test data for an cyclic uniaxial tension test with increasing strain levels.

Figure 2.24 highlights a few observations that are typical for the softening of elastomers. Most of the softening happens after the first loading and only occurs for stretches lower or equal to the maximum stretch previously applied. Residual strain upon unloading has also been attributed to softening. After a few cycles , the stress responses coincide with the
following cycles, the material behaviour stabilizes. When the stretch exceeds the former maximum then the stress curve returns to the primary loading path. Softening increases progressively as the strain maximum is increased.

Softening has been reported for various states of deformations but the exact mechanical quantity that governs it is still unclear.

Softening appears to be more eminent in elastomers containing filler material, such as carbon-black fillers, where a material with a higher filler content is prone to softening at lower stretch levels than elastomers with low filler content. It has been shown that the softening can be recovered under elevated temperature or solvent exposure. At room temperature, however, the recovery is negligible. Hence, many material models in literature, which are mostly phenomenological, consider softening as a damaging process. Many softening damage models multiply the classic strain energy function used in hyperelasticity (see Section 2.7.1) with a reducing factor:

\[
\Psi(F) = (1 - d)\Psi_0(F) .
\]  

where \(d\) defines a damage (polymer chain damage, microstructural damage etc), \(\Psi\) the strain energy function and \(F\) the deformation gradient. Models vary in terms of damage criteria (whether \(d\) changes or not in terms of the mechanical variables characterizing it) and damage law (how \(d\) changes). There are two basic approaches, one in which the stress-strain response of the second loading is identical to the unloading stress-strain response as long as the maximum strain is not exceeded (idealized response) and one where this is not the case. In the first case, the damage is only a function of a discontinuity, such as maximal applied strain. In the second case, the damage is also a function of a continuous variable that accumulates over the deformation process. Models of the first type are often preferred for simplicity. Details of these phenomenological models have been reported by Diani et al. [112]. Phenomenological models can deliver reasonable results as long as permanent set
and induced anisotropy are neglected.

Various researchers attempted to define physical explanations for the softening phenomenon. Some of the explanations include rupturing of chemical bonds, slipping molecules, filler rupture and disentanglement of polymer chains. The work by Diani et al. contains an overview of some physical models [112].

Abaqus uses a material model similar to the approach in equation 2.60 [13]. It is based on a hyperelastic material model with a strain energy function, \( \Psi \), that is not only a function of the deformation gradient but also of a damage variable. \( \Psi \) is not only the stored energy potential here, since part of the energy is dissipated by damage. The energy function is decoupled into deviatoric and volumetric parts (as seen before in Section 2.7.1) and is augmented with the damage function. The damage variable is a continuous function that changes during the course of the deformation.

**Elasticity Tensor**

Apart from defining a constitutive model, it is necessary to define the elasticity tensor in order to obtain solutions of nonlinear problems in finite elasticity and inelasticity [12]. Commonly, incremental/iterative solution techniques of Newton’s type are employed to solve a sequence of linearized problems. This technique can only be applied when the linearized constitutive equation is known.

The material tensor of elasticity, \( C \), describes the change in stress resulting from a change in strain

\[
dS = C : \frac{1}{2} dC ,
\]

where \( dS \) is the incremental change of the second Piola-Kirchhoff stress tensor and \( dC \) is the incremental change of the right Cauchy-green tensor. \( C \) is the gradient of the second
Piola-Kirchhoff stress and is defined as follows:

\[
C = 4 \frac{\partial^2 \psi(C)}{\partial C \partial C} = 2 \frac{\partial S(C)}{\partial C} = 2 \frac{\partial S(E)}{\partial E}.
\]  

(2.62)

The elasticity tensor is a fourth order tensor that is symmetric for all elastic materials. It possesses so-called minor symmetries

\[
C_{ABCD} = C_{BACD} = C_{ABDC}
\]

(2.63)

and for hyperelastic materials it also possesses the major symmetry

\[
C_{ABCD} = C_{CDAB},
\]

(2.64)

resulting in a fourth order tensor with 21 independent components at each strain state. As seen in the Section 2.7.1, the elasticity tensor may also be decoupled into a volumetric component, \(C_{vol}\), and an isochoric component, \(C_{iso}\), where former is defined as

\[
C_{vol} = 2 \frac{\partial S_{vol}}{\partial C}
\]

(2.65)

and the latter as

\[
C_{ISO} = 2 \frac{\partial S_{ISO}}{\partial C}.
\]

(2.66)

Using a proper structure for the elasticity tensor is crucial for the FE method in order to preserve quadratic rate of convergence near the solution point, when the Newton method is used. The elasticity tensor described here is defined within a consistent linearization process of the associated stress tensor, where the consistent linearization means a linearization of all quantities related to the nonlinear problem. The elasticity tensors in equations 2.65 and 2.66 are often called consistent linearized tangent moduli.

It is often simpler to use numerical tangent moduli due to the difficulties involved in
deriving the analytical linearized tangent moduli. One possible approach to compute a numerical tangent moduli is a method, in which the deformation gradient, $F$, is perturbed as it has been described by Miehe [114].

2.7.2 FE Modeling Approaches for Elastomers

What deformation behaviour of an elastomer is modeled depends on its application. Considering nonlinear elasticity (hyperelasticity) is sufficient when single loadings of a material are considered. However, when the unloading is also of interest, then hysteresis needs to be taken into consideration. Viscoelasticity, or time-dependency has to be included when the deformation behaviour over an extended time is of interest. In the case of cyclic loading, softening may also be considered if it is present in the material being investigated. As described in Section 2.7.1, the deformation behaviour of an elastomer under cyclic loading usually reaches a stabilized state. Hence, if the initial behaviour is not of interest and the material is loaded for many cycles, then it is suitable to use the stabilized loading and/or unloading stress-strain curve with a hyperelastic and/or hysteresis model.

In Abaqus, different standard material models can be considered, such as hyperelasticity that comes with a hysteresis option, and time-dependency. Softening can also be accounted for, but not simultaneously with time-dependency [13].

Another approach is to use more advanced polymer models such as the Bergstroem-Boyce model [115, 116] or the Qi-Boyce model for PU [11]. These models divide the deformation into a nonlinear elastic component and a nonlinear viscoelastic/plastic component. Figure 2.25 shows a 1D rheological representation of such a model. The model consists of the elastic component represented by a nonlinear spring and the time-dependent component represented by a linear spring and a nonlinear dashpot, which adds the time-dependency.

The model makes use of the fact that deformation gradient, $F$, is equal in both parts

$$F_E = F_V \ .$$ (2.67)
Furthermore, the deformation gradient of the viscoplastic part, $F_V$, can be separated, via a multiplicative decomposition, into an elastic, $F_{eV}$, and a viscoplastic contribution, $F_{pV}$:

$$F_V = F_{eV} \cdot F_{pV} \quad (2.68)$$

Furthermore, the time-dependency of the viscoplastic part is described with a distinct constitutive equation.

Some of these more advanced models also include softening effects. One such example is the previously described QB model [11]. Qi et al. attributed the softening to gradual release of initially in hard segments occluded soft segments during deformation. Hence, the softening (damage) function attempts to model these changes in soft and hard segments. More details are presented by Qi et al. [11].

An overview of different approaches to model TKRs using FEA will now be presented.
2.8 Computational Modeling of TKRs

Various different modeling approaches have been used in the literature to estimate kinematics, contact pressures, stresses and even wear in TKRs. Two basic concepts are usually employed: dynamic and (quasi-) static simulations. In the static approach, discrete moments in time are investigated. It is often used to compare different loading scenarios and TKR designs. In 2008, D’Lima et al. built an FEA knee model consisting of a rigid femoral component and tibial tray and a deformable tibial UHMWPE inlay [117]. They calculated contact pressure and area for kneeling and lunging. The relative positions of the components were derived from fluoroscopic kinematic data, and axial forces measured using an instrumented tibia were applied at discrete positions. In a study from 2005 by Morra et al., stair climbing, rising from a chair and deep knee flexion were investigated [118]. They positioned the rigid femoral component relative to the deformable UHMWPE inlay and applied axial compression and AP forces found in the literature in order to calculate contact pressure in different knee designs. The same group has also compared various knee designs by applying an axial force at full extension, mimicking heel strike, using a knee model that does not include any soft tissue effects [119–121].

Dynamic TKR models usually only consist of rigid bodies in order to minimize computational time and the contact mechanics (pressure and area) are estimated using softened contact definitions between the rigid bodies by defining a pressure-overclosure (elastic foundation) relation. These kinds of models allow the accurate simulation of the knee kinematics, while at the same time outputting contact pressure and area. Sometimes, the inlay is modeled as a deformable body. In 2003, Fregly and colleagues evaluated a rigid, dynamic model with a deformable body contact (elastic foundation) by comparing kinematics and contact pressures to an experimental study [122]. There are two different approaches presented in the literature to dynamically simulate TKRs in FEA programs: completely displacement driven and mainly force driven simulations. An example of a completely displacement
driven simulation is part of the work by D'Lima et al., who apply this method to the TKR components kinematics derived from fluoroscopy gait cycle and high flexion activity data, together with axial forces occurring during gait and high flexion activities, calculated using an instrumented tibia [117]. They found that high flexion activities such as lunging and kneeling produce much higher contact stresses than walking. Force driven simulations, in which loads are applied to control the kinematics, seem to be more common. Godest et al. (2001) developed a TKR model consisting of a rigid femoral component and a deformable UHMWPE inlay in which an axial and anterior/posterior load, internal/external torque and femoral component flexion occurring during a gait cycle were applied, to estimate knee kinematics and inlay stresses [123]. The loads were calculated from knee simulator results. The resulting kinematics of the two components in the FE model were then compared to the experimental kinematics from the simulator study. Simulated results were in good agreement with experimental results.

In 2005, Halloran et al. compared the kinematics and contact mechanics of a TKR during gait (force and flexion input from a knee simulator) using a completely rigid FE model with deformable contact and a deformable TKR FE model [124]. It was found that the rigid FE model results were reasonably close to the results of the deformable FE model at a fraction of the analysis time. Often, soft tissue is not included in these kinds of simulations; however, there are models that include ligaments. Halloran and colleagues developed a TKR FE knee model with femoral and patellar component and tibial inlay that also included certain ligaments [125]. Tibiofemoral loads and flexion angles derived from a knee simulator study as well as patella kinematics and quadriceps force measured in a human cadaver study were applied. Halloran et al. compared contact mechanics and kinematics of a rigid and deformable modeling approach with experimental results. The kinematics of both modeling approaches were in good agreement with experimental data and the contact mechanics of the rigid FE model showed acceptable correlation with the experimental data. The FE knee model described in this thesis also includes ligament effects, however, unlike
Halloran’s model, it does not individually model the ligaments, but rather simulates their effects as a whole (see Section 3.3.1).

There are also studies that report a combination of gait analysis with fluoroscopy to obtain relative TKR component positions used as input in a multibody dynamic model combined with a dynamic contact model (elastic foundation) and a computational wear model that models inlay damage as a combination of wear and creep, to predict clinical implant wear [126].

All of these FE simulation were conducted using conventional UHMWPE inlays. To the author’s knowledge, there have not yet been any FE simulations using PCU as an inlay material for TKR using an FE knee model.

The literature review presented in this chapter has described the important theory behind FE modelling, provided a summary of relevant background information and described some of the basic characteristics of the materials that will be considered in this thesis. In the next chapter, the materials and methods used to achieve the goals described earlier will be discussed.
Chapter 3

Materials and Methods

In the previous chapter, it was shown that various polymers are commonly used in orthopaedic implants to address clinical problems. PCUs have a long history of use in medical devices, and are a potential candidate material for use in orthopaedic implants. In order to predict the way in which PCUs will behave in an orthopaedic implant application, the mechanical behaviour must be investigated. The methods used to investigate this behaviour, and the materials investigated, will be described in this chapter. Additionally, this chapter will discuss the numerical modelling approach used to simulate the mechanical behaviour of PCU55D and PCU80A. In a next step a description of the FE knee model employed will be given.

3.1 Mechanical Experiments

3.1.1 Specimen Geometry

As described in Section 2.5.1, two PCUs with different hardness grades were investigated (PCU55D and PCU80A).

Circular and rectangular specimens were cut from “dog bone shaped” 4mm thick ISO 527-2 tensile specimens (see Figure 3.1) that were provided from a single industrial source. From
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Figure 3.1: Dimensions of the “Dog Bone Shaped” tensile specimen. All dimensions are in millimetres

Figure 3.2: “Dog Bone Shaped” tensile specimen, showing how cylindrical and rectangular specimens were cut out with a water jet. The scale shows four centimetres.

each tensile specimen, two 10 mm and four 8 mm diameter discs and three different rectangles (10x12.7mm, 10x10mm and 10x7mm) were cut (see Figure 3.2). The high elasticity of the material made it difficult to cut smooth and perpendicular edges without any bulging. It was found that cutting with a water jet delivered the best results. Specimens were only partly cut (see black arrows in Figure 3.2) in order to prevent losing them during the cutting process. These specimens were later fully cut using a scalpel.

3.1.2 Purpose and Type of Experiments

In order to assess the feasibility of PCU in TKRs, it is necessary to have a solid understanding of the general deformation behaviour of the polymer. For this thesis, it was decided
to focus on large deformation behaviour, deformation behaviour under longer term loading and softening behaviour. Large deformation in elastomers is commonly known as hyperelasticity, time-dependent behaviour is often described as viscoelasticity/plasticity, while softening may be referred to as the Mullins Effect (see Section 2.7.1). The main loading of a polymer insert in a PCL retaining TKR is compression; therefore it was decided to only assess the compressive response under compressive loading. The aforementioned deformation behaviours were investigated by performing the following experiments:

1. Cyclic unconfined compression at different strain rates (hereafter referred to as Test 1)
2. Cyclic unconfined compression with increasing strain level (hereafter referred to as Test 2)
3. Cyclic stepwise relaxation experiments (hereafter referred to as Test 3)

These experiments were selected to address the needs of the constitutive model which will be described later and to investigate the various behaviours mentioned above. Test 1 will reveal any strain rate dependency, Test 2 will show any possible softening during cyclic loading, and Test 3 will capture the time dependent deformation behaviour of the polymer. In order to validate the FE material model, it is necessary to show that the model is capable of predicting various deformation states. For this reason, the following additional experiment was performed:

4. Partly confined plane strain compression (hereafter referred to as Test 4)

All of the unconfined compression experiments were conducted using 8mm diameter discs, whereas the partly confined compression tests (plane strain) were performed using 10x7mm rectangles. The other specimens (10mm diameter discs, 10x10mm and 10x12.7mm rectangles) that were cut from the “dog bone shaped” tensile specimens were ultimately not required for testing and therefore discarded.
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3.1.3 Test Setup

To optimize time and the use of equipment at different testing laboratories, different tests were performed at different locations. Most of the unconfined compression tests and the plane strain experiments were conducted at Zimmer Inc., Warsaw IN, USA. In Zimmer Warsaw, the test setup consisted of an Instron 3345 universal testing machine (Instron, USA) with a 5kN load cell, a stainless steel water bath, a heating coil, and a thermocouple (see Figure 3.3(a)). Various relaxation and further unconfined compression tests were performed at Zimmer GmbH, Winterthur, Switzerland. In Zimmer Winterthur, a Zwick Z010 universal testing machine (Zwick, Germany) with a 10kN load cell and a transparent plastic water bath filled by circulating water pumped continuously from a thermostatically controlled heated reservoir, was used (see Figure 3.3(b)).

In both cases, the water bath was heated to 37°C, either directly or indirectly, in order to mimic the in vivo situation as close as possible, although to simplify testing, water was used instead of synovial fluid or Ringer’s Solution.
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3.1.4 Estimation of Reasonable Strain Levels

Typical loads in the knee during activities of daily living were found to be from 1-5 times body weight (see Section 2.1.3). Together with reported contact areas in commercial UHMWPE based TKRs ranging from 45 to 800mm$^2$ [127–132] and an average body weight of 83kg [133], contact stress could be calculated, although this resulted in a relatively large range of 1 to 90MPa. This broad range is a result of widely differing reported contact areas in TKRs, which have been experimentally measured [127–132] for different loadings, TKR designs and flexion angles. In literature, reported contact stresses are between 15 and 56MPa [117, 134, 135], and therefore approximately in the middle of the values calculated here. Both the PCUs considered here are very compliant at 37°C, therefore it is expected that TKRs with compliant inserts will have a larger contact area and therefore lower contact stresses. Consequently, it was decided to use a contact stress at the lower end of the calculated values in order to estimate reasonable strain levels for the mechanical experiments. A value of 35MPa was chosen as a representative stress. Subsequently, a pilot study was conducted, where the aforementioned PCU disks were compressed to roughly 90MPa, as can be seen in Figure 3.4, in order to obtain a first approximation of how the two PCUs behave under compression. A stress of 35MPa, as shown in Figure 3.4, results in a maximum strain of 60% and 80% for PCU55D and PCU80A respectively. These two values were subsequently used as maximum strain levels in all the tests.

3.1.5 Experimental Details and test Description

As described in Section 3.1.2, the test medium utilized was water heated to 37°C. The two test setups employed used different systems to keep the water at the desired temperature (see Figure 3.3). In Zimmer Warsaw (see Figure 3.3(a)), the water was heated directly in the specimen testing tank with a band heater attached to the outer wall of the tank. There was no water circulation present, but a stable water temperature due to the relatively small
mass of water required around the test apparatus was measured. In Zimmer Winterthur, however, a larger bath was used, hence, an external water reservoir with a heating coil was used which was connected to the tank by pipes (see Figure 3.3(a)). In this system, the heated water was circulated between the external reservoir and the testing water bath by a pump. The heating systems in both locations had controllers connected to a thermostat and in addition, manual measurements of the water temperature at the specimen location were performed periodically using a digital thermostat.

All specimens were preheated for two hours prior to testing and coated with a thin layer of Vaseline® in order to reduce friction between the specimen, the plunger and the test plate. Just before the start of each test the dimension of the specimen were measured using digital calipers.

All unconfined compression experiments (Test 1 to 3) were performed using a simple circular plunger and a base, as is illustrated in Figure 3.5(a), whereas Test 4 was performed using a die that constrains one of the lateral directions and a square plunger (see Figure 3.5(b)).

Figure 3.6 shows the test sequences of the simple unconfined compression (Test 1 as
seen in Figure 3.6(a)), unconfined compression with increasing strain levels (Test 2 as seen in Figure 3.6(b)) and relaxation (Test 3 as seen in Figure 3.6(c)), respectively. Figure 3.6(d) shows the test sequence of plane strain compression (Test 4). Experiments were conducted in displacement control mode and every step visible in Figure 3.6 corresponds to an increase or decrease in strain. In each experiment, a preload of 10N was applied in order to account for potential uneven surfaces and to ensure contact between the plunger and the specimen. All experiments, including the relaxation (Figure 3.6(c), only first cycle shown), were carried out for seven cycles in total. Cyclic loading was chosen because it shows how the stress-strain response changes over the cycles, revealing possible softening. A pilot study has shown that the material enters near steady-state, where the behaviour no longer significantly changes, after six to seven cycles, which corresponds with values found in literature [11, 89]. Hence, it was concluded that all tests should be run for seven cycles. A typical test would be performed as followed:

1. Heat water bath to temperature
CHAPTER 3. MATERIALS AND METHODS

2. Preheat specimen in water bath for two hours

3. Briefly remove specimens and measure dimensions

4. Apply Vaseline® to top and bottom faces of specimens

5. Place specimen in test apparatus

6. Start test sequence with preloading followed by actual test

In Test 1, simple unconfined compression test (Figure 3.6(a)), specimens were strained to a constant nominal strain of 60% for PCU55D and 80% for PCU80A, because this resulted in approximately equivalent loading regimes. The specimens were subsequently unloaded to 10N. These loading-unloading-cycles were repeated for seven times in total. Five different strain rates, $\dot{\varepsilon}$, were investigated, including 0.005, 0.01, 0.05, 0.1 and 0.3 s$^{-1}$.

In Test 2, unconfined compression with increasing strain levels (Figure 3.6(b)), PCU55D specimens were first cyclically loaded and unloaded seven times between 20% strain and 10N, then seven times between 40% strain and 10N and lastly between 60% strain and 10N for another seven cycles. PCU80A specimens were cycled between 20% strain and 10N, 50% strain and 10N, and lastly between 80% strain and 10N, all for seven cycles. For both materials, a 0.05 s$^{-1}$ strain rate was used.

In Test 3, relaxation (Figure 3.6(c)), specimens were subjected to several holding periods at different strain levels. PCU55D was first strained to 20% strain and kept at constant displacement for 30min, 33% strain for 30min, 47% strain for 30min and 60% strain for one second. Then the specimen was unloaded to 47% strain for 30min, 33% strain for 30min and lastly for another 30min at 20% strain. The same procedure was applied to PCU80A specimens but with strains of 20, 40, 60 and 80%. The stepwise strain increases were conducted at 0.1 s$^{-1}$ for both materials.

Specimens in Test 4, plane strain compression, were loaded in the same manner as the Test 1, however both PCU55D and PCU80A were stretched to the same maximal strain of
(a) Simple Unconfined Cyclic Compression (Test 1)  
(b) Unconfined cyclic compression with increasing strain level (Test 2)  
(c) Stepwise relaxation experiment (Test 3)  
(d) Plane strain compression (Test 4)  

Figure 3.6: Four different test sequences

60% (seven cycles), as can be seen in Figure 3.6(d), and only one strain rate was investigated (0.05 s$^{-1}$).

A total of 5 specimens were used for every experiment and material, except for the relaxation experiments for which 3 specimens were used. Table 3.1 provides an overview of all experiments conducted.

Part of the test data generated in these experiments will be used to model the deformation behaviour of PCU55D and PCU80A. The modeling will now be described.
### Table 3.1: Test overview and number of specimens used

<table>
<thead>
<tr>
<th>Type of Test</th>
<th>$\dot{\varepsilon}$ [$s^{-1}$]</th>
<th>Maximal $\varepsilon$ [%]</th>
<th>Hold Time [s]</th>
<th># Specimens</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test 1</td>
<td>0.3</td>
<td>60 (PCU55D)</td>
<td>na</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80 (PCU80A)</td>
<td></td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>0.1</td>
<td>60 (PCU55D)</td>
<td>na</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80 (PCU80A)</td>
<td></td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>0.05</td>
<td>60 (PCU55D)</td>
<td>na</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80 (PCU80A)</td>
<td></td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>60 (PCU55D)</td>
<td>na</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80 (PCU80A)</td>
<td></td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>0.005</td>
<td>60 (PCU55D)</td>
<td>na</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80 (PCU80A)</td>
<td></td>
<td>5</td>
</tr>
<tr>
<td>Test 2</td>
<td>0.05</td>
<td>20, 40, 60 (PCU55D)</td>
<td>na</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20, 50, 80 (PCU80A)</td>
<td></td>
<td>5</td>
</tr>
<tr>
<td>Test 3</td>
<td>0.1</td>
<td>20, 33, 47, 60 (PCU55D)</td>
<td>0.5h/step</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>20, 40, 60, 80 (PCU80A)</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>Test 4</td>
<td>0.05</td>
<td>60 (PCU55D)</td>
<td>na</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>60 (PCU80A)</td>
<td></td>
<td>5</td>
</tr>
</tbody>
</table>

Test 1: Cyclic Unconfined Compression; Test 2: Cyclic Unconfined Compression with Increasing Strain Levels; Test 3: Cyclic Stepwise Relaxation; Test 4: Plane Strain Compression
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3.2 Modeling of the Deformation Behaviour of PCU

In this section the constitutive model that was used to simulate the material behaviour, the curve fit routine required to obtain material specific coefficients and the validation procedure will be outlined.

3.2.1 Constitutive Model Used

Because only a vertical load was applied to the FE knee model (see results and discussion in Section 4.3 and 5.3), it was decided to just use a hyperelastic constitutive model. Hysteresis, softening and time-dependency will not influence a single, unrepeated loading.

Hyperelastic models which have been investigated, are mentioned in Table 2.6. It was found that the Yeoh model yields the best curve fit results for both PCUs. The curve fitting routine will be described in Section 3.2.2. A more detailed description of the Yeoh model, as found in the Abaqus manual [13], now follows.

The energy function used by Abaqus is similar to that in Table 2.6. However, Abaqus employs a version for almost incompressible materials where the energy function is decoupled into an isochoric and a volumetric part. It is defined as follows:

$$\Psi = \sum_{i=1}^{3} C_{i0}(\bar{I}_1 - 3)^i + \sum_{i=1}^{3} \frac{1}{D_{i0}} (J_{el} - 1)^2 i.$$  \hspace{1cm} (3.1)

Here $C_{i0}$ and $D_{i0}$ are 6 material coefficients, where $D_1 = \frac{2}{K_0}$ with $K_0$ being the initial bulk modulus. $\bar{I}_1$ is the deviatoric first strain invariant where the volume change has been eliminated. $\bar{I}_1$ is defined as the trace of the deviatoric left Cauchy-Green strain tensor, $\bar{B}$:

$$\bar{I}_1 = \text{trace}(\bar{B})$$  \hspace{1cm} (3.2)
where $\bar{\mathbf{B}}$ is a calculated from the deviatoric deformation tensor, $\bar{\mathbf{F}}$

$$
\bar{\mathbf{B}} = \bar{\mathbf{F}}\bar{\mathbf{F}}^T = J^{-2/3}\bar{\mathbf{F}}\bar{\mathbf{F}}^T \quad (3.3)
$$

$\bar{I}_1$ can also be defined in terms of the principal stretch. For uniaxial deformation, the relation is defined as:

$$
\bar{I}_1 = \lambda_u^2 + 2\lambda_u^{-1} \quad , \quad (3.4)
$$

where $\lambda_u$ is the stretch in the deformation axis.

The Yeoh model depends only on the first invariant, $\bar{I}_1$, since the sensitivity of the strain energy function to changes in the second invariant, $\bar{I}_2$, are usually much smaller than the sensitivity to changes in $\bar{I}_1$. Moreover, the sensitivity of $\bar{I}_2$ is difficult to measure and it was found that if data of only one deformation mode is available, omission of $\bar{I}_2$ dependence might enhance prediction.

Taking the derivative of equation 3.1 with respect to principal stretches, yields the following nominal stress function for incompressible materials:

$$
P = 2(\lambda_u + \lambda_u^{-2})\sum_{i=1}^{3} iC_{i0}(\bar{I}_1 - 3)^{i-3} \quad . \quad (3.5)
$$

To use the Yeoh Model in Abaqus, the material constants $C_{i0}$ and $D_{i0}$ ($i = 1, 3$) must be provided. In case of incompressibility, the coefficients $D_{i0}$ need to be set to zero. An individual perturbation study of the $C_{i0}$ coefficients revealed the influence that each of the three values has on the stress-strain relationship. The individual perturbation results are presented in Figure 3.7. Note that the origins of the curves in the Figure 3.7 are at zero strain and stretch equal to 1. In Figure 3.7(a), it can be seen that varying $C_{10}$ results in changes in the initial slope of the curves without influencing the response at higher stretches. Conversely, $C_{20}$ changes the slope of the last 2/3 of the stress-stretch curve (see Figure 3.7(b)) and $C_{30}$ changes the slope of just the last third resulting in more or less
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Figure 3.7: Figures a-c show the dependence of the stress response on the three Yeoh model coefficients $C_{10}$, $C_{20}$ and $C_{30}$. Green curves indicate positive values of the Yeoh model coefficients and red curves indicate negative values, while the blue curve indicates a value of zero of the Yeoh model coefficients.
negative curl as can be seen in Figure 3.7(c).

Next, the curve fit routine to obtain the three material coefficients will be described.

### 3.2.2 Curve Fit Routine - Material Coefficient Determination

Using the built-in curve fit tool did not yield satisfying curve fit results (low \( R^2 \) values). Therefore, it was decided to write a Matlab (Mathworks, Natick, MA, USA) code to perform the curve fitting. Matlab offers several nonlinear curve fitting algorithms. In this work, a function that curve fits data in a least-squares sense, called \textit{lsqcurvefit}, was employed. \textit{lsqcurvefit} requires a user-defined function, in this case the stress relation from equation 2.19. In addition, the x- and y-data must be provided in vector form, where in this case x-data are experimental uniaxial stretch data and y-data are experimental nominal stress values. For the design variables, or coefficients \((C_{10}, C_{20}, C_{30})\) that need to be determined, initial values must be specified. It was found that \textit{lsqcurvefit} is a very robust algorithm and initial values were not very important. If required, upper and lower bounds of all coefficients can also be defined.

A description of the data preparation that was necessary in order to use the mechanical test data in the curve fitting routine is now described.

#### Data Preparation

As described in Section 3.2.1, only hyperelastic material behaviour was considered in this report. Therefore, only loading data of one cycle from the uniaxial compression tests could be used (see Test 1 in Table 3.1). Due to the cyclic loading nature in the knee, it was decided to use the stabilized loading curve (7\textsuperscript{th} loading cycle), which has also been previously suggested by Geary \textit{et al.} to be appropriate [89]. Hence, this loading cycle was extracted from the complete data set and stress and strain values were subsequently shifted to zero. In addition to shifting the data to the origin, the data was also adjusted to a new initial length and contact area. Figure 3.8 shows an example of how the test data was adjusted.
Figure 3.8: Left: Entire test data with 7th cycle loading highlighted in red; Right: Extracted 7th loading curve

The stabilized loading curve was extracted and adjusted for each test and specimen using a Matlab program to automatize the process and the curve fit routine was used to determine the three coefficients. Apart from visually inspecting the curve fits, an $R^2$ value was calculated using the following equations:

$$R^2 = 1 - \frac{SSE}{SST}$$  \hspace{1cm} (3.6)

where $SSE$ is the sum of squared errors and $SST$ is the total sum of squares calculated as follows:

$$SSE = \sum_i (y_i - f_i)^2$$  \hspace{1cm} (3.7)

$$SST = \sum_i (y_i - \bar{y})^2$$  \hspace{1cm} (3.8)

Here, $y_i$ are the observed values, $f_i$, the modeled values and $\bar{y}$, the mean of the observed values.

Using the material parameters of all tests, a mean value and standard deviation was calculated for $C_{10}$, $C_{20}$ and $C_{30}$, for both PCU55D and PCU80A. The mean values for PCU55D and PCU80A were then used in the FE knee simulation (see Section 4.3). In addition, lower and upper boundary values were calculated for the three coefficients by
adding or subtracting the standard deviation from the mean values. These lower and upper values for both PCUs were used in one knee simulation in order to assess their influence on certain results (see Section 4.3).

Using the material coefficients presented here, validation simulations were performed. The validation procedure of these simulations will now be presented.

### 3.2.3 Validation Procedure

In order to assess how well the mean, lower and upper material coefficients obtained from the curve fits, match the actual experimentally determined material behaviour, a simulation of the uniaxial compression tests was performed in Abaqus. The test setup was modeled using axisymmetric elements, making use of the symmetry of the setup and the disk specimens, in order to make the computation more efficient. The half disc was meshed with 400 2D linear, quadrilateral hybrid elements of type CAX4RH (axisymmetric). Hybrid, or mixed formulation elements are used in Abaqus to deal with numerical instabilities that may occur when using conventional, purely displacement based elements in conjunction with incompressible materials [13]. The plunger was modeled as a rigid line, and frictionless contact was assumed between the two components. A displacement of -1.46mm and -2.15mm for PCU55D and PCU80A, respectively, in accordance with the experimental results, was applied to the rigid plunger. Three different sets of material coefficients (mean, upper and lower boundary values) were used for both PCUs. They are summarized in Table 3.2 (see also Section 4.2.1).

Resulting strain and nominal stress were then compared to the experimental data of all tests and specimens. Using the same coefficients shown in Table 3.2, the plane strain experiments were also simulated. The test cubes (see Section 3.1.1) were modeled using 4800 3D linear, hexahedral hybrid elements of type C3D8RH. The plunger and the die walls were modeled as rigid surfaces and contact between the specimen and the die and plunger surfaces was set to be frictionless. Similarly to the simulations described above,
Table 3.2: Yeoh Model Coefficients - Mean, upper and lower boundary values

<table>
<thead>
<tr>
<th>Value</th>
<th>PCU55D Coefficients</th>
<th>PCU80A Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( C_{10} )</td>
<td>( C_{20} )</td>
</tr>
<tr>
<td>mean</td>
<td>4.94</td>
<td>-0.55</td>
</tr>
<tr>
<td>upper boundary</td>
<td>5.59</td>
<td>-0.18</td>
</tr>
<tr>
<td>lower boundary</td>
<td>4.29</td>
<td>-0.93</td>
</tr>
</tbody>
</table>

a displacement in accordance with experiments was applied to the plunger and resulting strain and stress compared to the experiments. Since the material coefficients were derived from stabilized loading curves, the stabilized loading curve of the plane strain experiments was used for comparison. The curves were extracted in the same manner as described in Section 3.2.2.

So far, the mechanical testing procedure used to determine the deformation behaviour of the two polymers and the material deformation behaviour modeling have been explained. This information will be used as the basis of the FE knee model which will be presented next.

### 3.3 FE Knee Model Simulations

For this work, a dynamic FE knee model developed by Zimmer (Zimmer GmbH, Switzerland) was used to simulate certain physiological relevant knee joint loadings. The knee model allows the simulation of the positions of the knee components during a gait cycle [136, 137].

In order to assess the feasibility of PCU in TKR, two different approaches (Approach I and II) were considered. In a first step, Approach I, a modified, implicit version of the original explicit FE knee model was used in Abaqus/Standard (Version 6.8-1, Dassault Systèmes Simulia Corp., Providence, Rhode Island). It includes the application of an axial
force (and an AP displacement in some cases) at different discrete flexion angles followed by an analysis of the contact area, contact stress and von Mises stresses in the tibial inlay. Since it was considered interesting to investigate the performance of the polymer inlay over a continuous set of flexion angles, a second approach, Approach II, was also considered. Approach II consists of two steps. First, it uses the original FEA knee model to dynamically simulate a gait cycle in Abaqus/Explicit. Secondly, the kinematic output (the position of TKR components) of the dynamic simulation will then be used as input for an implicit quasi-static displacement-driven simulation in Abaqus/Standard, in which the motion of the components occurring during gait is retraced and the contact area, contact stress and von Mises stresses in the tibial inlay are subsequently analyzed.

This section provides a short explanation of the original knee model, as described elsewhere [136, 137], and then outlines changes that were applied to it in order for it to be used in the different approaches. The material properties of UHMWPE were also used in the same model to compare to the performance of PCU material properties in this model.

### 3.3.1 The Original Explicit FE Model with TKR

The knee model was built in Abaqus/CAE. The Abaqus package includes two different solver approaches, Abaqus/Explicit and Abaqus/Standard [13]. The former allows the simulation of dynamic problems, whereas the latter is used in static and quasi-static simulations. Both solvers are also capable of solving various other physical problems, but these will not be discussed here, as these other capabilities are not applicable to this work.

The main intended application of the original FEA knee model is to simulate the gait cycle, and so may be solved using Abaqus/Explicit. The original model consists only of rigid bodies in order to make it computationally more efficient and is composed of 3D bodies of the proximal ends of the femur and tibia bone, including articular cartilage, derived from sagittal magnetic resonance images (MRI) of a left, fully extended knee. For the purpose of this study, the articular cartilage was replaced by a TKR (NexGen® CR-Flex, Zimmer
Figure 3.9: Example of the NexGen® CR-Flex TKR, ©Zimmer GmbH

GmbH) consisting of a femoral component, a tibial tray and a tibial insert. The design used is cruciate ligament retaining and offers an optimized design that can accommodate high flexion of up to 155° [138]. Figure 3.9 shows an example of the employed prosthesis. The complete FE knee model package used includes a function that allows the virtual implantation of a TKR [137].

Figure 3.10(a) a shows the original FE knee model with bones and cartilage components and Figure 3.10(b) shows the corresponding model with a TKR, which for the original model, consists of a femoral component, a tibial inlay and a tibial tray. The original model does not include the menisci, although, the collateral and cruciate ligaments are included via a custom made joint elasticity function (JEF). The JEF is a phenomenological approach to model the passive soft tissue of a knee joint, relating the tibiofemoral relative position in six degrees of freedom (DOF) to an overall resultant soft tissue force and moment and therefore approximating the constraining effects of the passive soft tissues. The joint elasticity function is implemented as a linear neuro-fuzzy model and was calibrated/trained using specific training data obtained during robotic manipulation of a human knee joint from which the femoral condyles and tibial plateaus had been removed. The joint surfaces were removed in order to exclude any geometry effects. In this way, the JEF includes passive soft tissue effects only and can also be used with TKRs. In the original knee
(a) FE knee model without TKR seen from a medial anterior (left) and medial posterior view (right)

(b) FE knee model with TKR seen from a medial anterior (Left) and medial posterior view

Figure 3.10: FE knee model
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model, the JEF is linked to the femur and tibia and acts as a nonlinear six DOF boundary condition depending on the relative tibiofemoral position. This has been described in more detail previously [136, 137]. In the TKR model used here, the JEF is linked to the TKR components.

In addition to the force and moment resulting from the JEF, forces and moments as well as displacements resulting in the knee motion occurring during a gait cycle, were applied (see Section 3.3.3). These inputs are according to the ISO standard 14243-1 gait cycle [14].

Meshing of Components

To optimize the computation, only components that are relevant for this work are included in the FEA simulation, hence only the femoral component and the tibial inlay are meshed. The bone segments are not included in the analysis and therefore not meshed.

Both the femoral and the tibial component are meshed with rigid shell elements with a thickness of 0.001mm. The tibial inlay surface (without the bottom) and the articular surface of the femoral component are meshed with linear quadrilateral (type S4R) and linear triangular (type S3R) elements with an average global element size of 2mm. The inlay surface consists of 1646 elements and the femoral component contains 1516 elements.

Constraints and Contact Definition

The FE knee model contains four different coordinate systems (CSs), two for each component (tibial and femoral). There are two anatomical CSs, which are defined using anatomical landmarks, and are hereafter referred to as JEF CSs. The second set of CSs, which will be referred to as ISO CSs, are in accordance with the ISO definition [14]. A more detailed description of the four CSs is available in Appendix B, in which Figure B.1 shows all the CSs.

As described above, the TKR components are defined as rigid in order to make the computation more efficient. In a rigid body, the relative position of nodes within the body
remains constant, e.g. there is no deformation present. In order to use a rigid body, a reference point (RP) needs to be defined to which all the loads and boundary conditions are applied. For the femoral component, the ISO femur RP is used, which coincides with the ISO CS origin of the femur. Similarly, the ISO tibia RP is used for the tibial component. It coincides with the origin of the tibial ISO CS. In addition to RPs, so-called tie nodes may be defined, which have translational and rotational DOFs associated with the rigid body. The tie nodes of the femoral component and the tibial component are the JEF RPs that coincide with the origin of the femoral JEF CS and the origin of the tibial JEF CS, respectively.

To define the articular surface contact, a surface-to-surface contact type with finite sliding and penalty contact algorithm was employed. The penalty contact algorithm allows contact between rigid bodies. The femoral articular surface is defined as the master surface, while the tibial inlay articular surface is defined as the slave surface, indicating that the femoral articular surface is allowed to penetrate the tibial articular surface. This kind of contact formulation approximately resembles a deformable contact in the normal direction. The behaviour of the contact in the normal direction is defined with a pressure-overclosure relation that is based on the elastic foundation principle (bed of springs). In this method, the contact layers of known thickness are represented by scattered elastic springs that are independent of each other. In Abaqus, the pressure-overclosure can be supplied in tabular form, relating penetration to contact pressure. In literature, different elastic, nonlinear elastic and viscoelastic foundation models can be found. All of these models described were applied to compressible materials (Poisson’s ratio, \( \nu \), less than 0.5). Researchers have used elastic foundation models to analyse contact mechanics [122, 124, 139], predict wear [126] and simulate kinematics [124, 125] in TKRs. The original FEA knee model with TKR used in this thesis, is intended for conventional UHMWPE tibial inlays. Hence, it uses a pressure-overclosure relation derived for PE, which describes the normal contact pressure, \( p \), as a function of compressive modulus, \( E_c \), Poissons’ ratio, \( \nu \), normal penetration, \( u \),
and layer thickness, \( b \), as can be seen in equations 3.9 and 3.10 for small and large surface deformation, respectively [140].

\[
p = \frac{(1 - \nu)E}{(1 + \nu)(1 - 2\nu)} \frac{u}{b} \tag{3.9}
\]

\[
p = -\frac{(1 - \nu)E}{(1 + \nu)(1 - 2\nu)} \ln\left(1 - \frac{u}{b}\right) \tag{3.10}
\]

An average inlay thickness of 10mm was used for \( b \), which seems to be typical of the thickness of inlays in commercial TKRs.

The Poisson’s ratio of the PCUs investigated in this thesis was initially set to be 0.5, assuming incompressibility, as it has also been done by Qi et al. [11]. This causes calculation errors when using it with equations 3.9 and 3.10. The denominators contain the term \((1 - 2\nu)\), which, when \( \nu = 0.5 \) is used, become zero, resulting in division by 0. This causes the pressure to become \( \infty \), therefore making it necessary to reduce the Poisson’s ratio that was selected for the model, in order to allow the model to function correctly. The largest Poisson’s ratio that still allowed the gait simulations to work, was \( \nu = 0.495 \). This was not an issue for the simulations using UHMWPE, because the Poisson’s ratio of UHMWPE is 0.46.

In addition to the normal behaviour, the tangential contact behaviour has to be defined. The coefficient of friction (COF), \( \mu \), for PU against metal (lubricated, pin-on-disk) found in literature ranges from 0.003 to 0.035 [88, 94]. Here, a constant \( \mu = 0.02 \) was used.

Using a rigid approach with deformable contact definition does not yield any internal stresses and strains, however it is, if only contact mechanics are desired, much more efficient than running an explicit simulation with deformable bodies.

The mesh, constraints and contact definition, loading conditions and material properties of the implicit model used in Approach I shall now be described in turn.
3.3.2 Approach I - Simulations Using a Modified, Implicit Model with TKR

In order to assess PCU in TKRs it is of value to not only know the contact mechanics (contact area and pressure) but also stresses and strains within the polymer inlay. Unlike in Abaqus/Explicit, simulating deformations in Abaqus/Standard is not as computationally expensive. The original model from Section 3.3.1 was used as a basis. The main difference is the fact that an implicit solver is used. Moreover, all the functions and properties associated with the JEF were removed, as they are not applicable in Abaqus/Standard. However, all the CSs and reference points described above, were carried over. Due to the high compliancy of PCU80A, it is thought that the fixation of a pure PCU80A inlay to the tibial tray may be problematic. Therefore, a double layer inlay consisting of a compliant PCU80A articular layer (minimum thickness of 2.5mm) on a stiffer PCU55D substrate was modeled. This complies with reports found in literature (see Section 2.4.3) which describe a tibial inlay with two layers, a stiffer substrate and a more compliant articulation layer. Employing a simple "graded" inlay with different material properties may bring the TKR closer to the articular cartilage structure of the natural knee. In the FE model, the two layers are both deformable and connected via a tie contact definition that rigidly connects neighbouring surface nodes. The stiff substrate layer in turn is tied to the rigid tibial tray which now uses the tibial ISO RP and tie node as described above to apply the loads and boundary conditions. An illustration of the FE TKR model employed is shown in Figure 3.11

Although PCU is the main material of interest for this work, UHMWPE will also be considered for comparison.

Meshing of Components

A h-refinement mesh convergence study, in which the number of elements is increased, was performed in order to ensure that the mesh size does not influence the desired results. The
Six different mesh sizes were investigated, ranging from 7300 to 305,360 number of elements (total number of all components). Figure 3.12 shows contact area, peak contact pressure and peak von Mises stress as a function of number of elements. From Figure 3.12 it can be seen that an increase of number of elements from 100,000 to 300,000 results in less than 1% change in contact area, 1.3% change in peak contact stress and 1.1% change in peak von Mises stress. Hence, it was concluded that a total number of elements of approximately 100,000 is sufficient.

The femoral component is modeled as a rigid body meshed with 3347 linear quadrilateral shell elements of type S4R and 99 linear triangular shell elements of type S3, all with an edge length of 1.5mm. The tibial component is no longer completely rigid. As in the deformable explicit model described in Section 3.3.3, the tibial component now consists of three separate bodies, the rigid tibial tray, a relatively stiff PCU55D substrate and the more compliant PCU80A articular layer. The rigid tibial tray is meshed with 3828 linear quadrilateral shell elements (S4R) and 95 linear triangular shell elements of type the S3, all with a global size
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Figure 3.12: Mesh size sensitivity of contact area, peak contact pressure and peak von Mises stress of 1.5mm. The substrate layer is meshed with 13,008 linear hexahedral elements of type C3D8RH and the more compliant PCU80A layer is meshed with 82,128 linear tetrahedral elements (C3D4H). The global element size is 1.125mm for both the substrate and the compliant layer. Due to the incompressibility of both polymers used in the two inlay layers, hybrid elements (mixed formulation) were used. Hybrid elements are used in Abaqus to deal with numerical instabilities that may occur when using conventional, purely displacement based elements in conjunction with incompressible materials [13].

Again, only the relevant geometries were included, hence the femoral and tibial segments were not meshed. Figure 3.13 shows the complete model with meshed components.

Constraints and Contact Definitions

The tibial tray and the femoral component are modeled as rigid bodies. This is legitimate since the compressive moduli of the two materials are orders of magnitudes higher than the moduli of all the PCUs considered in this report (see Section 3.3.2). This approach has also been reported in literature [117]. Also, the use of rigid bodies simplifies the application of loading. The femoral component is associated with the same RPs and tie nodes as the component in the original knee model, whereas the tibial tray uses the nodes that were
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Figure 3.13: FE TKR model with meshed components seen from a lateral posterior (left) and medial anterior view (right)

associated with the tibial inlay in the dynamic simulation. The more compliant PCU80A articulating layer is tied to the stiffer PCU55D substrate, which in turn is tied to the tibial tray.

A surface-to-surface contact with finite sliding is defined between articular surfaces of the femoral and tibial component, where the femoral articular surface is defined as the master surface and the tibial inlay articular surface is defined as the slave surface. For the normal behaviour, the default hard contact is used, while the tangential behaviour is described using a friction contact with $\mu=0.02$ for PCU (see section 3.3.1) and 0.04 for PE (this value has been reported previously in literature [123, 125]).

**Loads and Boundary Conditions**

For this version of the FEA knee model, no JEF loads are applied. As briefly described in Section 3.3, an axial load is applied at different flexion angles, without considering any other loads, except for high flexion activities, where an AP displacement is also applied. Five different loading conditions are considered. A body weight of 69.4kg was used for all loadings, which is the mean body weight reported by the three studies used here [23, 30, 102]. Morra et al. have also used a similar body weight of 71kg in their FEA study [118].

Three flexion angles occurring during the stance phase of gait, 15.83°, 10.15° and 5.17°,
corresponding to 17%, 28% and 38% of the gait cycle, respectively, are investigated. At 15.83°, the axial tibiofemoral load shows a first peak after heel strike (flat foot), 10.15° is the flexion angle where the load is lowest during the mid-stance phase and at 5.17° the load reaches another peak just before toe off. At these flexion angles, the knee is subject to axial tibial contact forces of 2.37BW, 1.59BW and 2.28BW, respectively, which are the largest loads occurring during a stance phase of gait as found by D’Lima et al. in 2006 [102]. Heinlein et al. and Zhao et al. have reported similar loads [24, 141]. Using the 69.4kg yields the following tibial-femoral forces of 1613.5N, 1082.5N and 1552.3N, respectively. Since D’Lima et al. [102] reported only percentage gait and not flexion angles, it was decided to use the corresponding flexion angles from the ISO gait cycle. [14].

In addition to these three gait cycle conditions, which are all at almost full extension, two higher flexion situations, stair climbing and squatting, were also investigated. While stair climbing is not a high flexion activity per se, higher flexion angles with similar forces compared to the stance phase of walking may occur. Squatting is a high flexion activity, which has previously been defined as activities requiring flexion angles of greater than 125° [142]. Smith et al. investigated tibiofemoral contact forces and kinematics during squatting and reported a flexion angle of 130° and an axial contact load of 30N/kg which results in an axial force of 2082N using a body mass of 69.4kg [23] and these were applied in this thesis. It was also decided to investigate the contact angle and axial force which are experienced during stair climbing. Costigan et al. measured tibiofemoral contact forces during stair climbing using a gait analysis and a subject specific knee model and an average axial contact load of approximately 29N/kg resulting in a contact force of 2012.6N and a flexion angle of approximately 56.6° were chosen [30]. This flexion angle represents the angle with the largest axial contact force occurring during stair climbing.

As the knee is flexed, the femur moves posteriorly with respect to the tibia. This effect, which is most prominent at higher flexion angles, is often referred to as femoral rollback. The static FEA knee model used, does not include soft tissue and relative movement of the
TKR component is therefore limited and only due to geometry effects. In order to account for the femoral rollback, an anterior force acting on the tibia was applied as has been previously reported by Morra \textit{et al.} [118]. However, this anterior force, which was taken from studies performed by D'Lima \textit{et al.} (2007) [143] and Thambyah (2008) [144], did not yield sufficient tibial anterior movement. Hence, a displacement was applied instead, in order to position the tibial inlay similarly to what is seen in radiographs in literature [15, 145].

Li \textit{et al.} measured passive and active healthy knee kinematics using a cadaver study at flexion angles of up to 150°. They reported anterior tibial movements of 24.5±11.4mm at 120° and 31.2±13.2mm at 150° [145]. In order to position the tibial inlay so that the femur is at the posterior edge of the inlay, the lower end values were used to estimate anterior movement at 130° flexion (linear interpolation) resulting in a value of 14.7mm. To simulate stair climbing an anterior tibial displacement of 8.9mm was applied which corresponds to the lower end of the translation reported by Li \textit{et al.} for 60° of flexion [145].

In a first step, a small axial load of 100N is applied to the tibial ISO RP to ensure proper contact between the two components. Then, the flexion is applied to the ISO RP of the femoral component (around the ISO CS x-axis) while at the same time the axial load is kept constant. Once the components are positioned, the actual axial load is applied to the ISO RP of the tibia in the positive direction of the tibial ISO CS z-axis. The AP displacement is applied along the positive direction of the tibial ISO CS y-axis.

Flexion is the only unconstrained motion of the femoral component. The tibial component is allowed to freely move, except for rotating about the flexion axis. Figure 3.14 illustrates the applied flexion, axial force and AP displacement and Table 3.3 summarizes all conditions investigated.

**Material Properties**

Since Approach 1 is a static simulation, no densities and inertias need to be defined. For the rigid femoral component and the tibial tray, elastic material properties for CoCr and
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Figure 3.14: Applied loads and displacement directions acting on a TKR

Table 3.3: Loading Conditions - Approach I

<table>
<thead>
<tr>
<th></th>
<th>Flexion [^{[\circ]}]</th>
<th>Axial Force [^{[N]}]</th>
<th>AP Displ. [^{[mm]}]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gait 1</td>
<td>15.83</td>
<td>1613.5</td>
<td>-</td>
<td>[14, 102]</td>
</tr>
<tr>
<td>Gait 2</td>
<td>10.15</td>
<td>1082.5</td>
<td>-</td>
<td>[14, 102]</td>
</tr>
<tr>
<td>Gait 3</td>
<td>5.17</td>
<td>1552.3</td>
<td>-</td>
<td>[14, 102]</td>
</tr>
<tr>
<td>Squatting</td>
<td>130</td>
<td>2082.3</td>
<td>14.7</td>
<td>[23, 145]</td>
</tr>
<tr>
<td>Stair Climbing</td>
<td>56.6</td>
<td>2012.6</td>
<td>8.9</td>
<td>[30, 145]</td>
</tr>
</tbody>
</table>

Gait 1: Heel Strike; Gait 2: Mid-Stance; Gait 3: Toe Off
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Table 3.4: Material properties of the tibial inlay obtained from curve fits of mechanical test data (see Section 3.2.2) - Approach I

<table>
<thead>
<tr>
<th>Property</th>
<th>PCU55D Value</th>
<th>PCU80A Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Coefficients</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{10}$ [-]</td>
<td>4.94</td>
<td>2.09</td>
</tr>
<tr>
<td>$C_{20}$ [-]</td>
<td>-0.55</td>
<td>0.12</td>
</tr>
<tr>
<td>$C_{30}$ [-]</td>
<td>1.49</td>
<td>0.34</td>
</tr>
<tr>
<td>Lower Bound Coefficients</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{10}$ [-]</td>
<td>4.29</td>
<td>2.04</td>
</tr>
<tr>
<td>$C_{20}$ [-]</td>
<td>-0.93</td>
<td>0.04</td>
</tr>
<tr>
<td>$C_{30}$ [-]</td>
<td>1.35</td>
<td>0.10</td>
</tr>
<tr>
<td>Upper Bound Coefficients</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_{10}$ [-]</td>
<td>5.59</td>
<td>2.14</td>
</tr>
<tr>
<td>$C_{20}$ [-]</td>
<td>-0.18</td>
<td>0.20</td>
</tr>
<tr>
<td>$C_{30}$ [-]</td>
<td>1.62</td>
<td>0.59</td>
</tr>
</tbody>
</table>

Table 3.5: Material properties of the femoral component and tibial inlay - Approach I

<table>
<thead>
<tr>
<th>Property</th>
<th>CoCr Value</th>
<th>Ti Value</th>
<th>UHMWPE Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_c$ [GPa]</td>
<td>200 [146]</td>
<td>110 [146]</td>
<td>0.45 [147]</td>
</tr>
<tr>
<td>$\nu$ [-]</td>
<td>0.3 [146]</td>
<td>0.3 [146]</td>
<td>0.46 [148]</td>
</tr>
</tbody>
</table>

Titanium, respectively, need to be defined, even though these properties will not influence the simulation results. Abaqus/Standard requires these in order to run simulations. The two layers of the tibial inlay are modeled as incompressible, hyperelastic materials defined by the Yeoh material model. The articular surface layer is modeled with PCU80A properties and the stiffer substrate with PCU55D properties. As described in Section 3.2.2, one loading condition was also tested with upper and lower bound coefficients to account for the variance in the test data. UHMWPE is modeled as a linear elastic material. Tables 3.4 and 3.5 list the material properties of all materials considered here.

Approach I was proposed to assess the performance of a PCU tibial inlay using a static FE knee model. Approach II which was proposed to assess the performance of a PCU tibial
inlay using a rigid dynamic FE knee model will now be described.

### 3.3.3 Approach II - Simulations Using an Explicit and Implicit Model

For the first part of Approach II, the original model described in Section 3.3.1, in which the mesh, contact definitions and constraints have already been described, will be utilized. In this section, the loads and boundary conditions, as well as the material properties, will be described.

#### Loads and Boundary Conditions - Explicit Model

Two sets of forces and moments, JEF loads and ISO gait cycle loads, are defined in the four different CSs described in Section 3.3.1. The JEF forces and moments (ligaments) are defined in the JEF CSs, whereas the ISO gait cycle loads are defined in the ISO CSs.

As presented in Section 3.3.1, all the forces, moments and displacements must be applied to reference points (RPs) which are associated with the rigid bodies that are subject to these inputs. The JEF loads and ISO gait cycle loads are applied to separate RPs, where the former loads are applied to JEF RPs (tie nodes) in the JEF CSs and the latter loads and displacements to the ISO RPs in the ISO CSs.

The simulation of the ISO gait cycle [14] using the FEA knee model requires two steps. In the initial position, the position of the knee model as defined by the implantation, the femoral and tibial component are not in an equilibrium position. Hence, before simulating the actual gait cycle, a settle step is introduced, where an axial force of 100N is applied to the ISO RP of the tibia in the positive direction of the tibial ISO CS z-axis. This ensures that the two components are in force equilibrium and that contact between the two is established. After this step, the actual gait cycle is applied.

Three force/moment inputs and one femur flexion input are applied [14]. The forces and moments, which include the AP-force, axial force and IE-torque (ISO tibial torque), are applied to the tibial ISO RP, whereas the femur flexion is applied to the femoral ISO
RP. Instead of applying the ISO gait cycle axial force $0.07 \times w$ (where $w = 82\, \text{mm}$, the tibial inlay width) medially of the tibial ISO CS z-axis (proximal/distal), as defined in the ISO standard gait cycle [14], it is more efficient to apply all of the forces and moments to the same RP. Thus, it is necessary to introduce an additional moment, which is due to this medial offset of the ISO axial force. Figure 3.15 shows the five ISO gait cycle inputs as a function of percentage gait cycle. The entire gait cycle is defined to last 1.1s [149]. The flexion angle, defined in radians, of the femoral component is applied about the ISO CS x-axis of the femur (see Figure B.1) and is the only DOF of this component. The AP-force is applied along the tibial ISO CS y-axis, the axial force is applied in the z-axis of the tibial ISO CS, the IE-moment is defined about the z-axis of the ISO CS of the tibia and the moment due to the axial force is applied around the tibial ISO CS y-axis.

Apart from the applied forces, moments and rotation of the ISO gait cycle, an additional boundary condition was defined, the flexion of the tibial component about the tibial ISO x-axis, which is fully constrained. All other motions of the tibial component are unconstrained [149].

**Material Properties**

In the case of a rigid FEA model, only the density, $\rho$, can directly influence the outcome of the simulation. Other material properties can only influence the results via the contact definition (see Section 3.3.1). Nevertheless, material properties need to be defined, as Abaqus/Explicit requires them in order to run simulations. For the purpose of this dynamic simulation, only elastic material properties were considered. In literature, PCU tibial inlays are usually made of two layers, consisting of a stiffer substrate and a compliant articular layer (see Section 2.4.3). However, in a rigid FEA knee model only one layer can be modeled. Therefore, the material properties of PCU80A, which is being considered for the compliant, articulating layer, are used. In addition, the elastic properties of CoCr must to be defined. For the model simulating UHMWPE instead of PCU, the material properties of the former
(a) Flexion angle
(b) Axial force - positive = proximal and negative = distal
(c) AP force - positive = anterior and negative = posterior
(d) IE torque - positive = internal and negative = external
(e) Moment about AP-axis - positive = valgus and negative = varus

Figure 3.15: Flexion and load input according to ISO gait cycle [14]
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Table 3.6: Material properties of the different TKR components - Approach II

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Property</th>
<th>Value</th>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_c$ [MPa]</td>
<td>12 †</td>
<td>$E_c$ [MPa]</td>
<td>450 [147]</td>
<td>$E_c$ [GPa]</td>
<td>235 [150]</td>
</tr>
<tr>
<td>$\nu$ [-]</td>
<td>0.495 ‡</td>
<td>$\nu$ [-]</td>
<td>0.46 [148]</td>
<td>$\nu$ [-]</td>
<td>0.3 [146]</td>
</tr>
<tr>
<td>$\rho$ [kg/m$^3$]</td>
<td>1190 [151]</td>
<td>$\rho$ [kg/m$^3$]</td>
<td>950 [152]</td>
<td>$\rho$ [kg/m$^3$]</td>
<td>7750 [153]</td>
</tr>
</tbody>
</table>

† derived from mechanical test data
‡ see Section 3.3.1

must also be defined. Table 3.6 lists the material properties of all materials considered here.

In a dynamic simulation, such as the simulation of a gait cycle, inertial properties of the model components must also be considered. As described earlier, only thin surfaces (shells) are included in the simulation and will therefore barely influence the motion of the knee. In order to account for the masses of the components that are not included in the simulation, such as the soft tissue and the bones, point masses are applied to the JEF RPs of the tibial component and femoral component. The mass applied to the tibial component is 4.9kg [149]. The motion of the femoral component is displacement-controlled and its mass does therefore not influence the overall motion. Nevertheless, an arbitrary mass of 0.4kg is applied in order to satisfy the needs of Abaqus/Explicit. Additionally, rotary inertias of 0.15t/mm$^2$ are applied to the femoral and tibial component [149], where the femoral rotary inertia does not influence the results.

For the second part of Approach II, the FE knee model used was the same as the one described in Section 3.3.2. The only differences are the applied loads and boundary conditions, which will now be defined.

**Loads and Boundary Conditions - Implicit Model**

For this version of the FEA knee model, no loads are applied. Instead, the kinematic output of the results of the model in the first part of Section 3.3.3 is used as input for
this model. Using a custom-built Matlab program, the motion of the tibial and femoral component occurring during the gait cycle are extracted (six DOFs) for the ISO RPs in the global Abaqus CS. With the same program, a step file for Abaqus/Standard is generated, where the six DOFs of the two components are defined as boundary conditions applied to ISO RPs in the global Abaqus CS. This file is then appended to the job input file of the implicit knee model described here. Then, the gait cycle is simulated, resulting in a displacement-controlled retracement of the gait ISO gait cycle.

No other boundary conditions need to be defined, since every DOF is controlled by the displacement input. For comparison, the original explicit FE knee model with a deformable inlay was also attempted. This variation of the first part of Approach II will now be outlined.

**The Use of Deformable rather than Rigid Components**

Instead of using rigid articular surfaces as described above in the first part of Section 3.3.3, the original explicit FEA knee model was changed so that it includes a deformable tibial inlay. This allows the assessment of the compliant tibial inlay over a continuous range of flexion angles with only one simulation.

According to compliant polymer TKR specifications found in literature (see section 2.4.3), the inlay was modeled consisting of a compliant PCU80A articular layer (minimum thickness of 2.5mm) on a stiffer PCU55D substrate. The two layers are connected via a tie contact definition that rigidly connects neighbouring surface nodes. The stiff substrate layer in turn is tied to the rigid tibial tray which now uses the tibial ISO RP and tie node described above to apply the loads and boundary conditions, which are identical in magnitude, direction and point of action as those described above. Instead of using the penalty contact algorithm with pressure-overclosure definition, a hard contact is used for the normal behaviour, while the tangential behaviour remains the same as above. The compliant articular layer of the inlay is meshed with 113,021 linear tetrahedral elements of the type C3D4 and the stiff substrate layer is meshed with 5469 linear hexahedral hybrid
elements of type C3D8R and 168 linear wedge hybrid elements of the type C3D6. The stiff substrate contains elements with an approximate global size of 1.5mm, whereas the approximate global element size of the elements of the compliant articular layer is roughly 1mm. The tibial tray is meshed with 1277 linear quadrilateral shell elements of type the S4R and 32 linear triangular shell elements of type S3R with a global size of 2mm.

The two polymer layers are modeled as incompressible hyperelastic materials defined by the coefficients of the Yeoh model (see section 3.2.1). Apart from the density, the following coefficients are used for the PCU55D (substrate) and the PCU80A (compliant layer):

1. PCU55D
   
   (a) $\rho = 1210\text{kg/m}^3$ [151]
   
   (b) $C_{10} = 4.94$, $C_{20} = -0.55$ and $C_{30} = 1.49$

2. PCU80A

   (a) $\rho = 1190\text{kg/m}^3$ [151]

   (b) $C_{10} = 2.09$, $C_{20} = 0.12$ and $C_{30} = 0.34$

In Abaqus/Explicit, solving deformable problems requires a lot of computational time, because of very small time increments, depending on the mechanical problem analysed. By increasing the density or using mass-scaling in which Abaqus increases the density of the chosen materials automatically depending on various criteria, either globally or locally, the minimum time increment needed can be increased. However, using mass-scaling or manually altering the density influences the accuracy of the simulation. Both methods were investigated in this work.
Chapter 4

Results

In this chapter, the results of the mechanical testing, the FE material modelling and the FE knee model simulation as described in Chapter 3 will be presented.

4.1 Mechanical Testing

In this section, the mechanical test results will be presented. Although they are presented as positive values, all stress and strains presented here describe compressive strain and stress.

4.1.1 Unconstrained Experiments - Complete Data Sets

The results of Tests 1-3, as introduced in Table 3.1 in Section 3.1.5, will now be presented. For each test, data of an individual specimen will be presented in order to highlight certain features, followed by an overview of all test data.

In Test 1, PCU55D and PCU80A specimens were subject to cyclic unconfined compression. Both materials show similar characteristics. In Figure 4.1, the results of one PCU55D specimen and one PCU80A specimen are shown. It can be seen that the stiffness of the materials increases with increasing strain, indicated by the increasing gradient of the
stress-strain curve.

This stiffening effect is more pronounced in PCU80A (Figure 4.1(b)), where the slope of the curve significantly changes at approximately 0.5-0.6 strain. PCU55D does not show such a large change in the slope, rather it continuously increases. Comparing Figure 4.1(a) with Figure 4.1(b) highlights that PCU80A is more compliant than PCU55D. For example, in order to achieve a stress of 10MPa, PCU55D must be strained to approximately 0.3, whereas PCU80A must be strained to approximately 0.5. Generally, for both materials, upon first loading to maximum strain (Section 3.1.5), the stress reaches its maximum value of the entire test and then upon unloading, a clear hysteresis can be observed. Also, some degree of residual strain, approximately 0.1, remains after unloading. The most distinct feature that is seen in Figure 4.1, is the difference between the loading curves, which is most prominent from the first to the second loading cycle. The gradient of the first loading curve is slightly smaller than the gradient in subsequent loadings. After each loading cycle, the maximum stress achieved decreases and the residual strain increases, however, the differences from one loading to the next, decrease with increasing number of loading cycles. Eventually, after six to seven cycles, residual strain and maximum stress remain almost constant and a stabilized state is reached. Further loading is not thought to significantly change the stress-strain curve.

As described in Section 3.1.2, PCU55D and PCU80A were tested at different strain rates. Figures 4.2 and 4.3 show the results of the cyclic unconfined compression tests (Test 1) conducted in Warsaw and Winterthur, respectively. The same features that have been described above, also apply for the rest of the test results presented in Figures 4.2 and 4.3. Overall, the individual tests show good repeatability between specimens (by visual comparison). Some of the differences between individual specimens observed are due to slightly varying maximum strain values applied. For example, in Figure 4.2(b), Specimen 5 was strained to a slightly higher maximum strain than the other specimens.

Results from Test 2 will now be presented. In Test 2, PCU55D and PCU80A specimens
(a) PCU55D: One specimen tested at $\dot{\varepsilon} = 0.1 \text{s}^{-1}$

(b) PCU80A: One specimen tested at $\dot{\varepsilon} = 0.1 \text{s}^{-1}$

Figure 4.1: Test 1: One specimen of $\dot{\varepsilon} = 0.1 \text{s}^{-1}$ unconfined compression test data for PCU55D (a) and PCU80A (b). Identical scales are used for ease of comparison.
CHAPTER 4. RESULTS

(a) PCU55D $\dot{\varepsilon} = 0.01 \text{s}^{-1}$

(b) PCU80A $\dot{\varepsilon} = 0.01 \text{s}^{-1}$

(c) PCU55D $\dot{\varepsilon} = 0.05 \text{s}^{-1}$

(d) PCU80A $\dot{\varepsilon} = 0.05 \text{s}^{-1}$

(e) PCU55D $\dot{\varepsilon} = 0.1 \text{s}^{-1}$

(f) PCU80A $\dot{\varepsilon} = 0.1 \text{s}^{-1}$

Figure 4.2: Test 1: Cyclic unconfined compression at different Strain Rates for PCU55D (a, c, e) and PCU80A (b, d, f). All specimens were tested in Warsaw. Identical scales are used for ease of comparison.
CHAPTER 4. RESULTS

(a) PCU55D $\dot{\varepsilon} = 0.3 \text{s}^{-1}$

(b) PCU80A $\dot{\varepsilon} = 0.3 \text{s}^{-1}$

(c) PCU55D $\dot{\varepsilon} = 0.01 \text{s}^{-1}$

(d) PCU80A $\dot{\varepsilon} = 0.01 \text{s}^{-1}$

(e) PCU55D $\dot{\varepsilon} = 0.005 \text{s}^{-1}$

(f) PCU80A $\dot{\varepsilon} = 0.005 \text{s}^{-1}$

Figure 4.3: Test 1: Cyclic unconfined compression at different strain rates for PCU55D (a, b, c) and PCU80A (d, e, f). All specimens were tested in Winterthur. Identical scales are used for ease of comparison.
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were subjected to cyclic unconfined compression with increasing strain levels. This test differs from Test 1 in that specimens were strained to more than one strain level. Figure 4.4 shows test results of one specimen for PCU55D and PCU80A. Many of the above described features of Test 1, such as difference between loading cycles, changing maximum stress and residual strain, can also be observed in the results presented in Figure 4.4. These features occur for each strain level. For example, in the case of PCU55D (Figure 4.4(a)), the specimen is first strained to 0.13 for seven cycles, during which the maximum achieved stress decreases, while the residual strain increases before the stress-strain behaviour reaches a stabilized state. Also, as seen previously, the first loading is significantly different from the subsequent loadings. Once the strain is increased to its new maximum of 0.33, the same characteristics reoccur. In this case, the stabilized state from the previous strain level is the basis from where the changes (for example in residual strain) happen. Further increase of the strain level to 0.52 once again results in increasing residual strain and decreasing maximum stress before a third equilibrium state is reached. The same behaviour is seen in PCU80A. It also appears that the amount of hysteresis (the area between loading and unloading curves) increases with increasing maximum strain level.

The cyclic unconfined compression tests with increasing strain levels (Test 2) were performed for a total of five specimens for each material. Figure 4.5 displays all the test results. All of the described characteristics also apply for all the other test data. As could already be seen for Test 1 data, the repeatability of individual specimens is fairly high with the main differences being the slightly differing maximum applied strains.

The last unconfined compression test that will be presented, is Test 3, cyclic stepwise relaxation. In Figure 4.6, the results of one PCU55D specimen and one PCU80A specimen are shown. In this test, the specimens were first compressed to a certain strain level and the displacement was subsequently kept constant for 30 minutes. Following this, the strain level was increased and again kept constant. A total of four strain increases were
(a) PCU55D: One specimen tested at $\dot{\varepsilon} = 0.05 \text{s}^{-1}$

(b) PCU80A: One specimen tested at $\dot{\varepsilon} = 0.05 \text{s}^{-1}$

Figure 4.4: Test 2: One specimen of cyclic unconfined compression with increasing strain levels for PCU55D (a) and PCU80A (b). Identical scales are used for ease of comparison.
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(a) PCU55D: One specimen tested at $\dot{\varepsilon}=0.05\,s^{-1}$

(b) PCU80A: One specimen tested at $\dot{\varepsilon}=0.05\,s^{-1}$

Figure 4.5: Test 2: Cyclic unconfined compression with increasing strain levels for PCU55D (a) and PCU80A (b). Identical scales are used for ease of comparison.

performed. Then, the strain level was stepwise decreased with intermediate holding periods of 30 minutes until the specimen was unloaded. As in Test 1 and 2, the loading and unloading sequence was repeated seven times. Generally, the same features and material behaviour differences as in seen Tests 1 and Test 2 were observed. The maximum strain level decreases and the residual strain increases with each cycle until a stabilized state is reached after six to seven cycles. However, unlike in the other tests, stress relaxation due to the intermediate holding periods can be observed. In Figures 4.6(a) and 4.6(b), the stress relaxation is represented by the vertical sections of the stress-strain curves. At these points during loading, the stress decreases, while the strain is kept constant. Conversely, during unloading, the stress increases while the strain is kept constant. The amount of stress relaxation (length of vertical line segments) increases with increasing strain level. During unloading the exact opposite happens. The amount of stress increase rises after strain reduction. It was found that after the 30-minute holding period the stress relaxation starts to reach a plateau, indicating that an equilibrium state would be reached if the holding period had been slightly longer. Three specimens were tested for each material. The data of all specimens is presented in Figure 4.7 and was seen to be fairly repeatable.
Figure 4.6: Test 3: One specimen of $\dot{\varepsilon} = 0.1\text{s}^{-1}$ cyclic stepwise relaxation experiments for PCU55D (a) and PCU80A (b). Identical scales are used for ease of comparison.
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(a) PCU55D \( \dot{\varepsilon} = 0.1 \text{s}^{-1} \)

(b) PCU80A \( \dot{\varepsilon} = 0.1 \text{s}^{-1} \)

Figure 4.7: Test 3: Cyclic stepwise relaxation experiments for PCU55D (a) and PCU80A (b). Identical scales are used for ease of comparison

These results have provided the basis for understanding how the two PCUs behave during cyclic unconfined compression. In the next section, the extracted stabilized loading cycles will be described.

4.1.2 Unconstrained Experiments - Stabilized Loading Curves

As described in Section 3.2, the stabilized loading curves were used to determine the Yeoh material coefficients. These data will now be presented. Figures 4.8 and 4.9 show the stabilized loading curves for each test condition tested in Warsaw and Winterthur, respectively.

Comparing the test results from specimens tested in Warsaw (Figure 4.8) with those from specimens tested in Winterthur (Figure 4.9) highlights that the individual test results from specimens tested in Warsaw are generally more repeatable than the results from specimens tested in Winterthur and the differences are more prominent for PCU80A (right column in Figures 4.8 and 4.9) than for PCU55D. Figure 4.10 illustrates the test with \( \dot{\varepsilon} = 0.01 \text{s}^{-1} \) that was conducted in both Warsaw and Winterthur. For PCU55D, which can be seen in Figure 4.10(a), the difference between results obtained in Winterthur and results obtained in Warsaw appears to be minimal. However, considering the slopes of the two sets reveals
Figure 4.8: Test 1: Stabilized loading of cyclic unconfined compression at different strain rates for PCU55D (a, b, c) and PCU80A (d, e, f) tested in Warsaw. Identical scales are used for ease of comparison.
Figure 4.9: Test 1: Stabilized loading of cyclic unconfined compression at different strain rates for PCU55D (a, c, e) and PCU80A (b, d, f) tested in Winterthur. Identical scales are used for ease of comparison.
that the stress-strain curves from experiments conducted in Warsaw are flatter and the stress achieved at the maximum strain is lower. Data from tests conducted in Warsaw shows that less stiffening at higher strains seems to occur in these tests compared to those conducted in Winterthur.

A comparison of all stabilized loading curve data tested at both locations is shown in Figure 4.11. What has already been observed for \( \dot{\varepsilon} = 0.01 \text{s}^{-1} \) test data, is also apparent when comparing all the test results. Stress-strain curves for both PCU55D and PCU80A tests conducted in Warsaw are flatter than stress-strain curves from tests conducted in Winterthur. Figure 4.11 also shows that stress-strain curves obtained in Winterthur show more scatter. Generally, PCU80A stress-strain curve are less reproducible than PCU55D curves.

These results are the basis for the material modeling. The constrained experiments will be presented next.
4.1.3 Constrained Experiments

In order to observe the deformation behaviour when specimens are partly constrained, plane strain compression tests were conducted. The results from these will now be described.

Test 4 is a plane strain compression test. As described in Section 3.1.5, specimens subjected to plane strain compression are physically constrained in one lateral axis during compression. In Figure 4.12, the test results are compared with the cyclic uniaxial compression test results (Test 1). In principle, the plane strain compression test results are very similar to the results from Test 1. After six to seven loading cycles, an equilibrium state is reached, in which the maximum stress and the residual strain no longer change. Hysteresis can also be seen. The main difference between Tests 1 and 4 is the stiffness of the stress-strain response. In the constrained, plane strain compression, the material behaviour is much stiffer than in the unconstrained test data, indicating that the stress achieved at similar vertical strains is much higher. This is true for both PCU55D and PCU80A. Also, as seen before, the deformation behaviour of PCU55D is significantly stiffer than the deformation behaviour of PCU80A.
(a) PCU55D plane strain compression versus cyclic unconfined compression

(b) PCU80A plane strain compression versus cyclic unconfined compression

Figure 4.12: Comparison of plane strain compression (Test 4) and cyclic uniaxial compression (Test 1) for PCU55D (a) and PCU80A (b). Identical scales are used for ease of comparison.
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(a) PCU55D plane strain compression

(b) PCU80A plane strain compression

Figure 4.13: Test 4: Comparison of plane strain compression test data for PCU55D (a) and PCU80A (b). Identical scales are used for ease of comparison.

Five specimens were tested for each of the materials. The repeatability is lower than in the other tests, as can be seen in Figure 4.12. This is especially true for PCU80A (Figure 4.13(b)).

The results presented in these sections have provided the basis for understanding how the two PCUs behave under various loading conditions. Part of these results have been used in the next section, which presents results of the FE material model.

4.2 FE Material Behaviour Modelling

In this section, the results of the curve fitting of the stabilized loading cycle will be presented. First, a comparison of representative curve fit results with their corresponding experimental data will be presented. Then, a few specific points regarding the quality of the curve fits will be highlighted. In Section 4.2.2, the results of validation simulations using the determined material coefficients will be presented.
4.2.1 Curve Fitting - Hyperelasticity

Generally, all the curve fits were in good agreement with experimental data ($R^2$ values of at least 0.99). Only representative examples of each test condition and material are presented since all the other curve fits are very similar. Figure 4.14 shows curve fits of one specimen of each strain rate tested in Warsaw and Figure 4.15 shows curve fits of the equivalent tests performed in Winterthur.

As stated above, the curve fits using the Yeoh model accurately describe the stress-strain behaviour for the load range tested. However, a closer look at lower strains shows some discrepancy between the curve fit and the experimental data. Figure 4.16(a) shows a comparison of the curve fit result with the experimental data for PCU55D. The measured stress-strain curve shows an initial steep rise (indicated by a black arrow) which starts flattening after less than one percent strain, before the gradient increases further. The curve fitted data does not capture this initial feature and instead its slope continuously increases with increasing strain. The maximum difference between curve fit and experimental data is 31% at 0.025 strain. After approximately 0.15 strain, the two curves meet and the difference thereafter remains very small. The same issue can also be seen for PCU80A in Figure 4.16(b). However, it is less distinct. Because the difference between the initial slope and the subsequent slope of the experimental stress strain curve is small, the maximum difference between curve fit and experimental data in PCU80A is slightly lower than in PCU55D. The differences reaches a maximum of 22% at 0.05 strain. The curve fit and experimental curve meet at a strain of approximately 0.25. The described discrepancy between curve fit and experimental data is observed in all data sets. This discrepancy did not greatly influence the over quality of the curve fit, since it is only a small portion of the the entire data.

In order to compare the test results from Warsaw with test results from Winterthur, the test with a strain rate of $\dot{\varepsilon} = 0.01 \text{s}^{-1}$ was conducted at both locations (Figures 4.14(a) and 4.15(c) for PCU55D and Figures 4.14(b) and 4.15(d) for PCU80A). Comparing the
Figure 4.14: Representative curve fit results of stabilized cycle tested in Warsaw at different strain rates for PCU55D (a, c, e) and PCU80A (b, d, f)
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(a) PCU55D $\dot{\varepsilon} = 0.005 \text{s}^{-1}$

(b) PCU80A $\dot{\varepsilon} = 0.005 \text{s}^{-1}$

(c) PCU55D $\dot{\varepsilon} = 0.01 \text{s}^{-1}$

(d) PCU80A $\dot{\varepsilon} = 0.01 \text{s}^{-1}$

(e) PCU55D $\dot{\varepsilon} = 0.3 \text{s}^{-1}$

(f) PCU80A $\dot{\varepsilon} = 0.3 \text{s}^{-1}$

Figure 4.15: Representative curve fit results of stabilized cycle tested in Winterthur at different strain rates for PCU55D (a, c, e) and PCU80A (b, d, f)
Yeoh coefficients of the two PCU55D tests revealed a statistically significant difference for the $C_{10}$ and $C_{20}$ coefficients ($p < 0.001$). In the case of PCU80A, all three coefficients are significantly different ($p < 0.05$). There was also a significant difference between some samples of both materials for some of the coefficients from tests with different strain rates. However, the differences were not consistent across the coefficients and it was not possible to conclude whether there was a distinct strain rate dependence.

The hyperelastic material model used in this work cannot account for strain rate dependence and so it was decided to use an overall mean value for all coefficients of both materials. To account for the existing variance in test results (see Section 4.1.2), lower and upper bound values for each coefficient were also calculated.

Table 4.1 lists the mean values of the Yeoh model coefficients of all tests with corresponding standard deviation. The individual coefficients of each test specimen are presented in Table A.1 in Appendix A.1. Using the mean coefficients of each test condition, an overall average and standard deviation (stnd) was calculated for $C_{10}$, $C_{20}$ and $C_{30}$. The mean coefficients and standard deviations are listed in Table 4.2. As described in Section 3.2.2, using the overall mean value and standard deviation, upper bound and lower bound coefficients could be calculated and these are also presented in Table 4.2.
Table 4.1: Curve fit results of Test 1 - Yeoh coefficients means and standard deviations (std)

<table>
<thead>
<tr>
<th>Test</th>
<th>PCU55D</th>
<th>PCU80A</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>C₁₀</td>
<td>C₂₀</td>
</tr>
<tr>
<td>0.3s⁻¹†</td>
<td>mean</td>
<td>4.89</td>
</tr>
<tr>
<td></td>
<td>std</td>
<td>0.33</td>
</tr>
<tr>
<td>0.1s⁻¹‡</td>
<td>mean</td>
<td>5.7</td>
</tr>
<tr>
<td></td>
<td>std</td>
<td>0.13</td>
</tr>
<tr>
<td>0.05s⁻¹‡</td>
<td>mean</td>
<td>5.54</td>
</tr>
<tr>
<td></td>
<td>std</td>
<td>0.19</td>
</tr>
<tr>
<td>0.01s⁻¹†</td>
<td>mean</td>
<td>4.23</td>
</tr>
<tr>
<td></td>
<td>std</td>
<td>0.14</td>
</tr>
<tr>
<td>0.01s⁻¹†</td>
<td>mean</td>
<td>4.95</td>
</tr>
<tr>
<td></td>
<td>std</td>
<td>0.09</td>
</tr>
<tr>
<td>0.005s⁻¹†</td>
<td>mean</td>
<td>4.40</td>
</tr>
<tr>
<td></td>
<td>std</td>
<td>0.29</td>
</tr>
</tbody>
</table>

† Tested in Winterthur, ‡ Tested in Warsaw

Table 4.2: Material coefficients - overall mean and standard deviation (std), upper and lower bound values of all tests combined

<table>
<thead>
<tr>
<th>Test</th>
<th>PCU55D</th>
<th>PCU80A</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>C₁₀</td>
<td>C₂₀</td>
</tr>
<tr>
<td>mean</td>
<td>4.94</td>
<td>-0.55</td>
</tr>
<tr>
<td>std</td>
<td>0.65</td>
<td>0.38</td>
</tr>
<tr>
<td>upper</td>
<td>5.59</td>
<td>-0.18</td>
</tr>
<tr>
<td>lower</td>
<td>4.29</td>
<td>-0.93</td>
</tr>
</tbody>
</table>
These curve fit results define the material models for PCU55D and PCU80A. These results will now be validated in two different FE simulations.

4.2.2 Validation of the FE Material Model

In this section, the obtained coefficients of the Yeoh model will be validated by simulating experiments using Abaqus. The results of the unconfined uniaxial test simulation will be presented first, followed by the simulation results of the plane strain compression.

Unconfined Uniaxial Compression - Test 1

The mean, lower and upper value Yeoh Coefficients were used to simulate the stabilized cycle of the uniaxial compression tests. Simulation results were compared to all PCU55D and PCU80A experimental data. Figures 4.17(a) and 4.17(b) compare the simulation results with the experimental data for PCU55D and PCU80A, respectively. The simulated stress-strain curve of PCU55D enclosed the spectrum of the experimental data, where the lower bound value simulation approximately coincides with the lowest gradient of the experimental curves, the upper bound value approximately coincides with the highest gradient of the experimental curves and the mean value simulation approximately lays between the lowest and highest gradient experimental curves. In the case of PCU80A, all the simulations and experimental data almost coincide for the first 0.2-0.25 strain. At higher strains, the lower bound value simulation follows the least steep test data curve and at strains higher than 0.45 the lower bound value simulation somewhat deviates from this curve, predicting slightly lower stresses than the least steep experimental data curve. The upper value simulation results do not follow the steepest experimental stress-strain curve, rather the simulation results coincide with one of the medium steep test curves.
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(a) Validation simulation results of PCU55D - Unconfined uniaxial compression

(b) Validation simulation results of PCU80A - Unconfined uniaxial compression

Figure 4.17: Stress-strain curves of unconfined uniaxial compression simulated in Abaqus using mean, upper and lower values of Yeoh coefficients; a: PCU55D and b: PCU80A
Plane Strain Compression - Test 4

The three Yeoh coefficient sets (lower bound, mean and upper bound) of PCU55D and PCU80A were used to simulate the plane strain experiments. Figures 4.18(a) and 4.18(b) show the comparison of the simulation results with the experimental data for PCU55D and PCU80A, respectively. For both materials, it is clearly visible that the simulation greatly overestimates stresses at higher strains, regardless of which coefficients are used. For PCU55D the maximum simulated stress value is approximately 110% larger than the experimental data and for PCU80A it is 820% larger.

Figures 4.18(c) and 4.18(d) show a more detailed view of the first 0.2 strain for PCU55D and PCU80A, respectively. As observed in the unconstrained uniaxial compression in Section 4.2.2, the PCU55D stress-strain curve in plane strain compression exhibits an initial steep slope followed by a leveling of the curve and later an increasing slope. The material model used is not able to predict this behaviour with any coefficient set. The simulation result using the mean coefficients is the closest to the experimental data. The simulated stress at 0.2 strain is 7% higher than the actual experimental data. The same situation for strains smaller than 0.2 for PCU80A is presented in 4.18(c). The experimental stress-strain curve is steeper than the simulated stress-strain curve in the beginning, then levels off before slightly increasing again. The trend of an initially steep gradient followed by leveling off of the stress-strain curve in PCU80A is, however, not as prominent as seen in PCU55D specimens. As in PCU55D simulations, the material model is not able to capture the initial slope changes. All three simulation results are close to the experimental data for strains below 0.1, but then deviate from the test data at higher strains. At a strain of 0.2, the maximum simulated stress is 48% larger than the experimentally observed stress values.

These curve fitting results show that the Yeoh material model is capable of predicting unconfined compression, but shows limitation for confined compression. The Yeoh model derived specifically for PCU55D and PCU80A was used in the FE knee model simulations.
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(a) Validation simulation results of PCU55D - Plane strain
(b) Validation simulation results of PCU80A - Plane strain
(c) Detailed view of validation simulation results of PCU55D - Plane strain
(d) Detailed view of validation simulation results of PCU80A - Plane strain

Figure 4.18: Stress-strain curves of plane strain compression simulated in Abaqus using mean, upper and lower values of Yeoh coefficients; a: PCU55D, b: PCU80A and c: Detail of PCU55D, d: Detail of PCU80A
The results of these simulations will now be discussed.

4.3 FE Knee Model Simulations

It has been shown possible to use various compression tests to gain a basic understanding of the mechanical behaviour of the PCU materials described here and subsequently this data has been used to tune the Yeoh material model. This material model will now be applied to a FE knee model simulation. Two different approaches were simulated, whose results will now be presented.

Since the proposed tibial inlay is composed of a layered structure consisting of PCU55D and PCU80A, the material will hereafter be referred to as PCU.

4.3.1 FE Knee Model Simulations Using Approach I

In Approach I, an implicit FE knee model with a deformable tibial PCU inlay was used to simulate different static knee loading scenarios (see Section 3.3.2).

Differences in Stress and Strain Using Lower, Mean and Upper Value Yeoh Coefficients

As described in Section 3.3.2, in order to assess the influence of different material coefficients and to account for the relative large variability in the test data (see Figures 4.8 to 4.11), it was decided to simulate one loading condition using upper and lower bound material coefficients. 5.17° of knee flexion was investigated which corresponds to toe off. Figure 4.19 shows a comparison of peak contact pressure, average contact pressure, peak von Mises stress and contact area for three different sets of material properties (lower bound, mean and upper bound).

Generally, the difference between lower, upper and mean values is relatively small. The difference between lower and upper bound for peak von Mises stress is 10.6%, for peak
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(a) Maximum von Mises stress

(b) Maximum contact pressure

(c) Average contact pressure

(d) Total contact area

Figure 4.19: Comparison of maximum contact pressure, maximum von Mises stress, average contact pressure and total contact area using mean, lower bound and upper bound Yeoh coefficients. The knee was flexed to 5.17°. One simulation was investigated per condition.
contact pressure is 6.3%, for the average contact pressure is 5.44% and for the contact area the difference is also 6.3%.

In the next section, the performance of PCU inlays during certain typical knee joint loading conditions will be compared to the performance of UHMWPE.

**Comparison of Contact Pressure, Contact Area and von Mises Stress in the PCU and UHMWPE Inlay**

In order to compare the performance of the PCU tibial inlay to the UHMWPE tibial inlay, four different descriptors were chosen and compared for each loading condition. For each of the five loading scenarios, total contact area, peak von Mises stress, peak contact pressure and average contact pressure were extracted. These values are summarized in Figure 4.20. Each descriptor is plotted as a function of flexion angle (flexion angles for walking are in the order as they occur during a gait cycle). In addition, the tibiofemoral contact forces that were used are also plotted as a function of flexion angle.

Generally, from Figure 4.20, it is clear that contact area decreases with increasing flexion angle, while von Mises stress and contact pressure (mean and average) increase with increasing flexion angle. The difference in von Mises Stress and contact pressures (Figure 4.20(b), 4.20(c) and 4.20(d)) for the walking loading conditions (15.83°, 10.15° and 5.17° of flexion) is small for PCU. For UHMWPE, 10.15° and 5.17° of flexion produce very similar maximum von Mises stress values and contact pressures. However, stress and pressure at 15.83° of flexion are significantly larger than in the other two walking load conditions, approaching values which occur during stair climbing. It is interesting to note that, for both materials, the walking condition in which the flexion angle is 15.83° predicts von Mises stress and contact pressure which are very similar to those occurring during stair climbing. Squatting produces by far the largest stress and pressure values, with contact pressure for UHMWPE reaching 57.1MPa, which is beyond the 8-15MPa [154–156] reported for UHMWPE compressive yield strength. The maximum contact pressure for PCU is 10.3MPa, which is
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Figure 4.20: Comparison of contact area, maximum von Mises stress, maximum contact pressure and average contact pressure found for PCU inlay and found for UHMWPE inlay at different flexion angles. Only one simulation per flexion angle was performed. Flexion angles for walking are shown in the order as they occur during a gait cycle.
significantly lower than in UHMWPE. A compressive yield strength of PCU could not be found, however, PCU80A was compressed to stresses of up to 60-70MPa in this project (see Section 4.1) and no permanent damage was observed. The maximum contact pressure of 10.3MPa for PCU is well below these values.

Contact pressure and von Mises stress observed in the PCU inlay are significantly lower than the values observed in the UHMWPE inlay. Accordingly, the contact area in PCU inlays is significantly higher than in UHMWPE inlays. Table 4.3 summarizes all the descriptor values for each loading and lists how much PCU values differ from UHMWPE values.

The simulated contact area for PCU is on average 345% greater than the contact area determined for UHMWPE. The greatest difference (437%) was found for squatting, while the smallest difference was recorded for 5.17° of flexion, where the contact area for PCU is 228% larger than the contact area for UHMWPE. As listed in Table 4.3, the relative difference between the PCU and UHMWPE inlay contact area increases with increasing flexion angle.

Peak von Mises stress, peak contact pressure and average contact pressure for PCU are on average 72% lower than for UHMWPE. Again, the largest difference is found for squatting. The average contact pressure at 130° of flexion is 70% lower for PCU than for UHMWPE, while the peak contact pressure is 82% lower. Generally, it can be said that, for all descriptors, the difference between the PCU inlay and UHMPE inlay increases with increasing flexion angle.

A comparison of contact pressure distributions in the PCU and UHMWPE inlay is now described. Only near full extension (5.17° of flexion) and squatting (130° of flexion) will be compared here. Other flexion angles are presented in Appendix B.2 for completeness. In Figures 4.21 and 4.22, contact pressure is compared for 5.17° and 130° of flexion for the PCU and UHMWPE inlay, respectively. The region with contact pressure, not considering actual values, is an indicator of the contact area. Comparing the regions between PCU
Table 4.3: Comparison of various descriptors between PCU and UHMWPE inlay; difference reported with respect to UHMWPE

<table>
<thead>
<tr>
<th>Activity</th>
<th>Flexion [°]</th>
<th>PCU</th>
<th>UHMWPE</th>
<th>Difference [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact Area [mm²]</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Walking</td>
<td>15.83</td>
<td>710.56</td>
<td>135.71</td>
<td>423.58</td>
</tr>
<tr>
<td>Walking</td>
<td>10.15</td>
<td>709.36</td>
<td>194.37</td>
<td>264.95</td>
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<tr>
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<td>5.17</td>
<td>851.99</td>
<td>259.81</td>
<td>227.93</td>
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<tr>
<td>Stair Climbing</td>
<td>56.60</td>
<td>536.13</td>
<td>114.28</td>
<td>369.16</td>
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<tr>
<td>Squatting</td>
<td>130.00</td>
<td>375.62</td>
<td>69.92</td>
<td>437.25</td>
</tr>
<tr>
<td>Peak von Mises Stress [MPa]</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Walking</td>
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<td>3.51</td>
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<tr>
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</tr>
<tr>
<td>Walking</td>
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<td>5.97</td>
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</tr>
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<td>73.81</td>
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<tr>
<td>Peak Contact Pressure [MPa]</td>
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<tr>
<td>Walking</td>
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<td>31.12</td>
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<tr>
<td>Walking</td>
<td>10.15</td>
<td>3.33</td>
<td>12.18</td>
<td>-72.68</td>
</tr>
<tr>
<td>Walking</td>
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<tr>
<td>Squatting</td>
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<td>57.10</td>
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<tr>
<td>Average Contact Pressure [MPa]</td>
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<td>Walking</td>
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<tr>
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<td>3.96</td>
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<td>130.00</td>
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<td>12.56</td>
<td>-69.75</td>
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</tbody>
</table>
(a) Contact pressure for 5.17° flexion - PCU Inlay

(b) Contact pressure for 5.17° flexion - UHMWPE Inlay

Figure 4.21: Comparison of contact pressure found in PCU and UHMWPE inlay for 5.17°. Scales are not consistent in all figures to more accurately illustrate the complete contact pressure distribution.
Figure 4.22: Comparison of contact pressure found in PCU and UHMWPE inlay for 130° flexion. Scales are not consistent in all figures to more accurately illustrate the complete contact pressure distribution.
inlay and UHMWPE for both flexion angles, visualizes the large difference in contact area reported in Table 4.3.

Comparing the posterior edged of the two inlays for a flexion angle of 130° (indicated by red arrows in Figures 4.22(a) and 4.22(b)), the PCU inlay (Figure 4.22(a)) is more deformed than the UHMWPE inlay (Figure 4.22(b)). The PCU inlay posterior walls are bulging out. This difference is not visible in the results for 5.17° of flexion (Figures 4.21(a) and 4.21(b)).

Comparing the 5.17° of flexion results with the 130° of flexion results highlights two points: Firstly, the area affected with contact pressure is more square like for almost full extension, especially for the PCU inlay, where the contact pressure distribution becomes more like a line contact at 130° of flexion. This especially true for UHMWPE. Secondly, the contact pressure distribution moves towards the posterior edge of the tibial inlay at 130° of flexion.

Some more specific results of the PCU tibial inlay will now be presented.

**Specific Results of the Performance of the PCU Inlay**

Figure 4.23(a) shows the undeformed tibial inlay. When loaded during squatting, the entire inlay is being pushed posteriorly (to the left of the modelled tibial inlay in Figure 4.23), resulting in von Mises stress concentration of approximately 4.5MPa around the substrate and tibial tray interface (Figure 4.23(b)). A closer examination confirms the bulging of the posterior wall of the inlay, as it can be seen in the highlighted section Figure 4.23(b).
In Figure 4.24(a), the position of the femoral component and tibial inlay at 130° of flexion is shown. It can be seen that the femoral component is at the posterior end of the tibial inlay. Although, the model does not include the femur, it is still clear that impingement between the posterior side of the femoral shaft and the tibial inlay may occur (see red arrow in Figure 4.24(a)). In Figure 4.24, the maximum principle strain distribution is plotted. The maximum strain value is approximately 0.38, occurring on the lateral tibial plateau where the femoral component contacts the inlay (see Figure 4.24(c)). In Figure 4.24(b) (highlighted area) and Figure 4.24(c) the large deformation and bulging of the posterior wall described above are also clearly visible. The squatting loading scenario presented here is the most demanding of all the load cases investigated.

The approach discussed here only allows discrete knee positions to be analyzed. A simulation of a complete gait cycle using the original FE knee model was also attempted, and these results will now be presented.

4.3.2 FE Knee Model Simulations Using Approach II

As described in Section 3.3.3, the aim of Approach II was to run an entire gait cycle using the original explicit FE knee model and then using the kinematic output to run an implicit, displacement-controlled simulation. This would allow continuous assessment of the tibial inlay, and the verification of Approach II is now described.

Validation of Approach II

In order to assess whether the implicit gait simulation using input obtained from explicit simulations functions correctly, a discrete gait event near full extension was compared to a simple implicit model in which an axial force is applied at full extension. The axial force used is 2400N which is similar to the force at the discrete gait event near full extension [14]. Figures 4.25 and 4.26 show a comparison of von Mises stress and contact pressure for a UHMWPE inlay, respectively. The contact pressure and von Mises pattern are similar in
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(a) Medial view of the femoral component and deformation of the tibial inlay at 130° of flexion
(b) Posterior view of the femoral component and deformation of the tibial inlay at 130° of flexion
(c) Top view of deformation of tibial inlay at 130° of flexion

Figure 4.24: Position of the femoral component and deformation of the PCU tibial inlay at 130° of flexion. Colour distribution indicates maximum principal nominal strain

both models. Peak contact pressure and von Mises stress are higher in the gait simulation, however, the stress and pressure in the main affected areas are similar (the stress and contact pressure are indicated by green colour). This simple comparison indicates that Approach II is valid for UHMWPE. The same comparison was performed for a PCU inlay. Due to the fact that only one material (PCU80A) can be modeled in the explicit FE gait simulation (“deformation” was achieved through pressure overclosure function), it was decided to use a full PCU80A inlay in the implicit, displacement-driven gait simulation. Hence the inlay of the simple implicit FE simulation with axial load was also modeled using PCU80A
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(a) Von Mises stress at 14° Flexion (2400N Axial Load)

(b) Von Mises stress: 2400N axial force applied at full extension

Figure 4.25: Comparison of von Mises stress between gait simulation using explicit FE knee kinematic input in implicit deformable FE knee model with implicit deformable FE knee model with similar load appliance. The knee is flexed to 14° for the gait simulation and fully extended for implicit static FE knee model. An axial force of 2400N is applied to fully extended FE knee model, which corresponds to force occurring in gait at 14° flexion. Scales are adjusted for ease of comparison.

- This model shows an UHMWPE Inlay
CHAPTER 4. RESULTS

(a) Contact pressure at $14^\circ$ Flexion (2400N axial load)

(b) Contact Pressure: 2400N axial force applied at full extension

Figure 4.26: Comparison of contact pressure between gait simulation using explicit FE knee kinematic input in implicit deformable FE knee model with implicit deformable FE knee model with similar load appliance. The knee is flexed to $14^\circ$ for the gait simulation and fully extended for implicit static FE knee model. An axial force of 2400N is applied to fully extended FE knee model, which corresponds to force occurring in gait at $14^\circ$ flexion. Scales are adjusted for ease of comparison.

- This model shows an UHMWPE Inlay
properties. This is different to the model investigated in Approach I which used a two layer construction of PCU55D and PCU80A. Figures 4.27 and 4.28 illustrate von Mises stress and contact pressure for the models, respectively. Figures 4.27 and 4.28 illustrate that the simulation with an axial force results in higher von Mises stress and contact pressure and the region of inlay affected is much larger. In the gait simulation, almost no contact between the inlay and the femoral component (see area affected with contact pressure in Figure 4.28(a)) is seen to occur. These differences are indicative of a lack of deformation in the implicit gait simulation. This implies that Approach II is not valid for the PCU investigated in this work.

To confirm the suspected lack of deformation, the kinematic output of the explicit gait simulation using a UHMWPE inlay was compared to the kinematics of the same simulation using a PCU80A inlay. It is clearly visible in Figure 4.29 that the kinematics using a UHMWPE inlay (pressure overclosure derived with UHMWPE properties) are very close to the kinematics using a PCU80A inlay (pressure overclosure derived with PCU80A properties). The PCU80A appears to move slightly more proximally during the gait cycle, although, the difference is small. Since the femur is fixed in this model, proximal movement of the tibial inlay could be an indicator of deformation occurring in the inlay. But again, if this is the case, it is a similar amount of deformation to that seen in the UHMWPE inlay. These findings further support the idea that Approach II does not work with PCU.

Explicit Simulation with Deformable Inlay

As described previously, it would be beneficial to be able to investigate deformation mechanics of the tibial inlay during the entire gait cycle. As an alternative to Approach II, which was shown to be inappropriate for PCU, the gait cycle was also simulated using a deformable version (inlay) of the dynamic FE knee model. This would allow the assessment of the compliant tibial inlay over a continuous range of flexion angles with only one simulation.
CHAPTER 4. RESULTS

(a) Von Mises stress at 14° flexion (2400 N axial load)

(b) Von Mises stress: 2400 N axial force applied at full extension

Figure 4.27: Comparison of von Mises stress between gait simulation using explicit FE knee kinematic input in implicit deformable FE knee model with implicit deformable FE knee model with similar load appliance. The knee is flexed to 14° for the gait simulation and fully extended for the implicit static FE knee model. An axial force of 2400 N is applied to fully extended FE Knee Model, which corresponds to the force occurring in gait at 14° flexion. Scales are identical for ease of comparison - This model shows a PCU80A Inlay
Figure 4.28: Comparison of contact pressure between gait simulation using explicit FE knee kinematic input in implicit deformable FE knee model with implicit deformable FE knee model with similar load appliance. The knee is flexed to 14° for the gait simulation and fully extended for the implicit static FE knee model. An axial force of 2400N is applied to fully extended FE Knee Model, which corresponds to the force occurring in gait at 14° flexion. Scales are identical for ease of comparison - This model shows a PCU80A Inlay.
A dynamic gait cycle simulation was attempted using the deformable inlay, however, simulations either did not finish or the results obtained were unrealistic due to excessive deformation and contact problems. The use of different mass-scalings was attempted but this did not resolve the problem.
Chapter 5

Discussion

In this chapter, some of the important findings reported in Chapter 4 will be discussed. The mechanical experiments will be discussed first, followed by a discussion of the FE material model and lastly, the outcome of the FE knee model simulations will be discussed.

5.1 Mechanical Testing

The results of the unconstrained compression experiments created in Tests 1, 2 and 3 will now be discussed.

5.1.1 Unconstrained Compression Experiments

Repeatability

It is important when simulating behaviour from experimental data that the tests are shown to be reasonably repeatable in order to accurately describe the behaviour of the material.

Generally, it was found that the qualitative repeatability of all the unconstrained compression experiments for the PCUs tested was good. However, there is some variability present in data obtained when testing PCU55D and PCU80A. As highlighted in Section 4.1.1, one reason for the inter-specimen variability is the fact that not all specimens were stretched.
to exactly the same maximum strain level. This is due to a combination of reasons. As defined in Section 3.1.5, specimens were pre-loaded before the actual test sequence was started. After pre-loading, strain and force were not zeroed, instead the tests were immediately started and the pre-load and resulting pre-strain were later adjusted during the data reduction. The maximum test strain was applied by defining a certain displacement based on the original length of the specimen and not based on the length after pre-loading. Therefore, post-experimental subtraction of the pre-strain varied among specimens, resulting in different maximum strain values. Other differences between samples are due to the normal material variability that is typically seen when mechanically characterizing polymers.

The issue described above is also present in the stabilized loading curves (Section 4.1.2), where the main variability appears to be the maximum strain achieved. Another reason for the variability observed in some cases, may be the varying residual strain upon unloading of the second last loading-unloading cycle. For example, if two specimens were strained to the same maximum amount, it is possible the extracted stabilized curves vary slightly, because of different residual strains of the previous loading-unloading cycles.

From the complete data sets of the cyclic unconfined compression test (Test 1), it was not possible to find distinct differences between test data obtained in Warsaw and test data obtained in Winterthur. However, comparing the stabilized loading curves revealed some differences. Generally, it seems that data obtained in Warsaw is more repeatable (see Figures 4.10 and 4.11). The exact reasons are not clear, since the same material batch and test procedure was used. The only difference is the equipment that was utilized. In Warsaw, a 5kN load cell was used which may provide greater accuracy than the 10kN load cell used in Winterthur for the load range that was tested (less than 2.5kN). Another possible reason for the difference could be that the test machine used in Warsaw more accurately applied the pre-loads. It is also interesting to note that the repeatability for PCU55D is greater than for PCU80A. It could be that PCU80A is more sensitive to slight changes in the test procedure, such as water bath temperature and applied strain. Another aspect that was
found to differ, is the amount of stiffening occurring at higher strains. Stress-strain curves from tests conducted in Winterthur exhibit greater stiffening at higher strains. This was first believed to be due to the different strain rates used, however, this difference is also present in the test which was performed at both locations using the same strain rate (see Figure 4.10). The cause for this difference is not understood.

Strain Rate Dependence, Hysteresis and Softening

Several different strain rates were used in order to investigate the strain rate dependence of PCU55D and PCU80A (Test 1). Usually, it is expected that the deformation behaviour of an elastomer stiffens with increasing strain rate. However, for the two materials investigated in this study, it was not possible to reveal a distinct strain-rate dependence (Figures 4.8 and 4.9). This might indicate that the deformation behaviour of the two materials is independent of the strain rate for the strain rate range investigated and so the strain rates might not be sufficiently different from each other to see distinct differences in behaviour. However, Qi et al. who investigated the compressive deformation behaviour of PCU 94A using similar strain rates ($\dot{\epsilon} = 0.01 \text{s}^{-1}$, $\dot{\epsilon} = 0.05 \text{s}^{-1}$ and $\dot{\epsilon} = 0.1 \text{s}^{-1}$), found some strain rate dependence [11]. However, unlike in this work, Qi et al. tested at room temperature. It might be possible that the material becomes less strain rate dependent at 37$^\circ$ and possible strain rate dependence may be masked by the material variability.

The features described in Section 4.1.1, such as hysteresis, residual strain and stabilizing deformation behaviour, are commonly observed in elastomeric materials. Elastomers usually show hysteretic behaviour during unloading, in which the stress during unloading is significantly lower than during loading. The hysteresis observed in PCU55D and PCU80A is relatively small compared to certain rubbers presented in literature [116]. When cyclically loaded, the stress-strain curve of an elastomer in the first loading cycle is often less compliant than the curve observed in subsequent cycles. This effect is known as the Mullins Effect, although this effect will be referred to in this discussion simply as softening. When
softening occurs, there is usually also some degree of residual strain present upon unloading and the maximum stress decreases after each cycle [112, 113]. Examining the data obtained in this study (see Figures 4.1 and 4.4), shows that some of the signs of softening occur. For example, as presented in Chapter 4.1, a residual strain of maximum 0.09-0.1 is present after the first loading/unloading cycle. Qi et al. reported residual strain of approximately 0.11 for PCU 94A [11]. The distinct difference between the first and second loading stress-strain curve as described in literature [112, 113], in which the second loading stress-strain curve is far more compliant (showing a smaller gradient in the stress-strain curve) than the first loading curve, is not visible in the data presented here. On the contrary, it appears that the gradients of the second and subsequent loading cycles are similar to, if not greater than, the gradient of the first loading cycle (see Figures 4.1 and 4.4). Similar observations can be made in the compression data of PCU 75D tested at $37^\circ$ reported by Geary et al. [89]. Test data for PCU 94A reported by Qi et al., shows the typically softening behaviour [11]. However, as described earlier, Qi et al. reported true stress-strain curves and tested at room temperature.

Another softening phenomena that can be seen in the data where the strain level is step-wise increased, which is also documented in literature [112, 113], is that once the strain level is increased beyond what was previously applied, the same features that occurred at the lower strain occur again. So, there is again a significant difference between the first and subsequent loading cycles; residual strain is present and the maximum stress achieved decreases with increasing number of cycles (see Figure 4.4). This agrees with what is reported in literature. According to the softening theory, the deformation behaviour normally stabilizes after a few cycles [112, 113]. In this work, it was found that the deformation behaviour of PCU55D and PCU80A stabilizes after six to seven cycles whenever the strain level was increased. This is in accordance with the theory and values reported in literature. For example, Geary et al., who conducted uniaxial tension tests, found that PCU80A stabilized after three loading-unloading cycles [89], while Qi et al. found that PCU 94A tested under compression,
stabilized after approximately four cycles [11].

Further experiments at different temperatures and more strain rates would be necessary to confirm whether the above rationale for the apparent lack of strain rate dependence, and softening is valid.

Relaxation

The step-wise relaxation experiments (Test 3) were performed in order to gain a better understanding of the time-dependent behaviour of PCU55D and PCU80A. Generally, the same features were observed for both PCU55D and PCU80A.

The amount of stress relaxation varies for each strain level. During loading, the amount of relaxation increases with increasing strain level, which can be seen by the increasing length of the vertical stress-strain curve sections shown in Figure 4.6. The different amount of relaxation during loading indicates that the relaxation is nonlinear and depends on the applied strain level. During unloading, the stress increases while the strain is kept constant, because upon strain reduction and subsequent holding, the specimen tends to continue expanding, but is hindered by the plunger which is fixed at a certain position. This constraint results in an increase in stress in the specimen with time. The amount of stress increase during the unloading holding periods grows with decreasing strain levels, which also indicates nonlinear viscoelastic behaviour.

Overall, it was found that the data obtained from testing PCU55D and PCU80A is of similar quality and shows the same phenomena. The main difference between the two materials for all experimental data, is the higher compliance of PCU80A, indicated by the smaller gradients and therefore lower stress at the same strain levels. It was also found that the observed features, such as hysteresis, residual strain and stabilizing deformation behaviour, which are typical for elastomers, were present in every experiment. However, the frequently mentioned softening under cyclic loading is not as distinct as in other elastomers and in some PCU data reported in literature. Also, no real strain rate dependence could
be found, even though it has been reported in literature. It was hypothesized that the elevated testing temperature of 37°C might be a possible cause for the difference between values reported in literature and test data reported here. The time-dependent behaviour was found to be nonlinear for both loading and unloading.

The constrained compression experiment will now be discussed.

5.1.2 Constrained Compression Experiment

In order to determine whether the FE material model is capable of simulating stress states other than purely uniaxial compression, plane strain compression (Test 4) was also performed.

The plane strain deformation behaviour (Figure 4.12) exhibits the same features as the unconstrained experiments. The only difference is the stiffer stress-strain response. Stresses at the same strain level as in unconstrained compression are significantly higher, which seems logical since one lateral movement of the specimen is fully constrained. The lateral expansion of the specimen is impeded by the die walls, which increases the stress in the specimen, because it cannot freely expand.

In a next step, the FE material model will be discussed.

5.2 FE Material Behaviour Modelling

In this section, the determination of the material coefficients via curve fitting routine and the validation of these coefficients will be discussed.

5.2.1 Curve Fitting of Stabilized Loading Curves

As described in Section 3.2.2, the stabilized loading cycles from the cyclic unconfined compression experiments (Test 1) were used to determine the hyperelastic Yeoh material coefficients. Generally, the quality of the curve fits was shown to be excellent for PCU55D and
PCU80A.

The representative curve fit results in Figure 4.14 and 4.15 illustrate the appropriateness of using the Yeoh model to model the data. The overall curve fit quality with $R^2$ values of at least 0.99 is excellent for both materials and the model is able to capture the deformation behaviour over a large range of strain. The quality of the curves fitted data obtained from testing PCU80A were generally better than the quality of curves fitted from data obtained from testing PCU55D. This is believed to be due to the fact that PCU80A shows more stiffening at higher strains than PCU55D, which is typical for hyperelastic materials. The stress-strain behaviour of PCU55D is closer to linear. The main deviation between material model predictions and experimental data occurs at strains of less than 0.25. In Section 4.2.1, it was observed that the Yeoh model is not able to capture the initial higher gradient in the experimental stress-strain curve followed by a decrease in stiffness (see Figure 4.16). This initial larger gradient may be due to a certain amount of stick-slip friction in lateral expansion occurring between the specimens and the test platens at the initiation of the compression. The friction may restrict the lateral expansion of the specimen which in turn may increase the force necessary to compress the specimen, hence increasing the stress experienced in the specimen. A purely elastic material model is likely to yield better results for the initial higher gradient than the hyperelastic Yeoh material model. However, a linear stress-strain curve would only be accurate for the first approximate 0.024 of strain and then would greatly deviate from the experimental data, resulting in differences much larger than those seen when using the Yeoh model. Therefore the use of a hyperelastic material model was considered to be valid, even though the experimental stress-strain nonlinearity during the first 0.25 of strain is limited.

It was hoped that by curve fitting the different stabilized loading cycles, a strain rate dependence could be detected. Instead, the obtained Yeoh coefficients listed in Table 4.1 confirm the visual comparison of all stabilized test data in Figure 4.11 that there is no apparent strain rate dependence. While a certain statistically significant difference between
some of the coefficients of the different strain rate experiments was found, it did not reveal a possible strain rate dependence. The slightly higher curve fit quality of PCU80A, indicated by higher $R^2$ values than found in PCU55D, is confirmed by the lower individual and overall standard deviations of the Yeoh coefficients (see Tables 4.1 and 4.2).

The curve fit results confirmed that the Yeoh model is appropriate for predicting the stabilized stress-strain behaviour during loading of PCU55D and PCU80A. Statistical analysis of the individual curve fit results supported the visual observations of the stabilized loading curves that no apparent strain rate dependence is present.

The application of the Yeoh coefficients in FE simulations will now be discussed.

5.2.2 Validation of the Yeoh Material Model Coefficients

In order to assess whether the Yeoh model derived from uniaxial test data is able to predict the deformation behaviour of PCU55D and PCU80A, certain experiments were simulated in Abaqus.

Using the mean, lower and upper bound Yeoh coefficients (see Table 4.2) the stabilized loading cycle data was simulated in Abaqus. The hyperelastic material model cannot account for different stress-strain behaviours, e.g. only one data set from one stress-strain curve can be considered for each model. By using mean, lower and upper bound Yeoh coefficients it was possible to account for the variability found in the test data. As seen in Figure 4.17, the three simulations enclose the various experimental stress-strain curves, showing that the combination of the three coefficient sets account for all experimental data.

To assess whether the Yeoh material model is able to predict the stress-strain behaviour of a multiaxial stress state, planes strain compression was also simulated. The simulation results for plane strain compression are generally in poor agreement with experimental data (see Figure 4.18). The simulation overestimates stress at higher strains. The accuracy at strains below 0.15 to 0.20 is acceptable. Considering that strains found in the FE knee simulations close to the interface of substrate and tray, where the inlay is constraint
the most, are less than 0.25 (see Section 4.3.1), the Yeoh material model derived here, is expected to still deliver valid results. The maximum simulated strains occurring in the inlay are approximately 0.38 on the articular contact surface. This area is considered to be mostly unconstrained. The exact reasons for the hugely overestimated stresses at higher strains could not be determined. Using the obtained Yeoh coefficients to simulate unconstrained compression (Test 1) exceeding the maximum strain applied in the experiments, showed that the stress rapidly increases with only a slight increase in strain greater than the experimental range. It is possible that in plane strain compression, this rapid increase in stiffness occurs sooner than observed during the plane strain experiments. As described in Section 3.2.3, the rectangular specimen was modelled using linear elements. Quadratic elements may yield more accurate results for incompressible materials where the deformation is partly or fully constrained. It may be that the linear elements are responsible for the overestimation of the stress at higher strains, where the incompressibility of the material would be especially eminent. Hybrid (mixed formulation) elements were used to enhance the linear elements, making them more suitable for incompressible materials. Hybrid elements are used in Abaqus to deal with numerical instabilities that may occur when using conventional, purely displacement based elements in conjunction with incompressible materials [13]. However, using linear hybrid elements alone may not be sufficient.

The simulation of the plane strain compression has shown that further investigations may determine how the the hyperelastic material model is able to estimate multiaxial stress states. It might be necessary to use additional load cases (biaxial, shear loading etc) to derive the material coefficients. It might even be necessary to look into a more advanced material model such as the Qi-Boyce [11] or Bergstroem-Boyce model [157]. The latter is especially true if a more dynamic and long-term material deformation behaviour is of interest.

In the next section, the results of the application of the Yeoh material model to an FE knee model will be discussed.
5.3 FE Knee Model Simulations

5.3.1 FE Knee Model Simulations using Approach I

In Approach I, an implicit FE knee model with a deformable tibial PCU inlay was used to simulate different static knee loading scenarios (see Section 3.3.2).

Differences in Stress and Strain Using Lower, Mean and Upper Value Yeoh Coefficients

Taking into account the material behaviour variability seen in the uniaxial compression tests (see Section 4.1.2), one loading condition, 5.17° of flexion, was simulated using computed lower and upper bound Yeoh coefficients in addition to the overall mean values (see Section 4.3.1). Comparison of the different results, such as contact area or contact pressure, showed that the difference between the results obtained using the three different material coefficient sets, is relatively low.

The largest difference (10.6%) between lower and upper bound values was found for peak von Mises stress. Using this difference, it can be assumed that all the FE knee simulation reported in this thesis, which were obtained using the overall mean material coefficients, should be within a ± 5% range of values.

Using an overall mean Yeoh coefficient set was shown to be a valid approach with the available mechanical test data and constitutive material model.

The comparison of the FE knee model results with data from literature will now be discussed.

Comparison of Tibial Inlay Contact Pressure and Contact Area to Simulation Results Presented in Literature

FE knee simulations with an UHMWPE inlay were performed in order to be able to compare the performance of the new compliant PCU inlay to an existing product. The results of the
UHMWPE simulations and the PCU simulations will now be compared to those presented in literature.

Documented compressive yield strength values of UHMWPE range from 8-15MPa [154–156]. As listed in Table 4.3, the contact pressure determined for the UHMWPE inlay ranged from 11MPa at almost full knee extension to 57MPa at 130° of flexion. Maximum contact pressures of flexion angles greater than 15° are well in excess of the compressive yield strength of UHMWPE and even the lower contact pressure values are very close to the maximum compressive yield strength reported in literature. However, the average contact pressure found in this study ranges from 3.43-12.56MPa which lays within the range of compressive yield strengths of UHMWPE.

The maximum contact pressure in the PCU inlay reported in this report is 10.3MPa. This is well below the compressive stresses investigated in this project. PCU80A was tested to up to 60-70MPa without permanent damage (see Section 4.3.1), which may be an indicator that the risk of abrasive wear of the PCU articular surfaces investigated in this thesis is minimal.

Experimentally determined contact pressures for UHMWPE TKRs, as determined by pressure films, range from 10-38MPa, depending on design and loading condition [127, 129, 131]. These values compare well with those reported in this study (11-57MPa). Various FE studies have also investigated contact pressure in UHMWPE inlays. Morra et al. investigated the same UHMWPE based prosthesis used here and reported a maximum contact pressures of 20-26MPa at full extension [120]. These values are higher than the one found in this report (11MPa), however the axial load used by Morra et al. was approximately 500N higher. Godest et al. have reported maximum contact pressures during gait of 23MPa occurring at a flexion angle of approximately 15° [123], whereas Halloran et al. reported a contact stress of 20-30MPa at a similar angle [124, 125]. These values are slightly lower than what was found in this thesis (31MPa). D'Lima et al. reported contact pressures for stair climbing of 27MPa which is slightly lower than what is reported in this thesis (32.7MPa)
The same group reported a contact pressure of 58MPa for lunging (120° of flexion) which is very close to the contact pressure for squatting reported in this study (57MPa).

Contact areas for UHMWPE inlays reported in literature range from 80-300mm$^2$, depending on axial load, flexion angle and design [117, 129, 131]. The range of contact area for UHMWPE found in this report is 70-260mm$^2$ which compares well with the range reported in literature. Using FEA, Halloran et al. determined contact areas of 250-300mm$^2$ for a flexion angle of approximately 15° [125], which is approximately twice as much as presented in this report. Morra et al., reported a contact area of 242mm$^2$ for full extension [120]. This is very close to the 259.8mm$^2$ reported in this project.

Generally, contact pressures and contact areas reported for UHMWPE in this study compare well with experimental and computational values found in literature and any differences are most likely due to slightly different loading conditions, UHMWPE material models, FE knee model formulation (rigid vs deformable) and different implant designs. These comparisons support the validity of Approach I for UHMWPE.

Contact area of the natural knee has been reported to vary between 765-1150mm$^2$ [117]. In this study, the contact area for a PCU inlay was found to be between 376-852mm$^2$, which is relatively close to the natural knee. It appears that using a compliant polymer results in a TKR that is closer to what is observed in nature. It is a first step towards a more natural solution.

The comparison of contact pressure, contact area and von Mises stress in the PCU and UHMWPE inlays will now be discussed.

Comparison of Contact Pressure, Contact Area and von Mises Stress in the PCU and UHMWPE Inlay

In Section 4.3.1, contact pressure, contact area and von Mises stress in the PCU tibial inlay were compared to the results of the conventional UHMWPE inlay. The most important differences found are the significant increase in contact area and subsequent decrease in
contact pressure. As the flexion angle increases, the congruency between the femoral component and the tibial inlay decreases, resulting in a decrease in contact area and increase in contact pressure. The issue of low congruency is especially visible in the UHMWPE inlay at 130° of flexion (see Figure 4.22). At 130° (see Figure 4.22(b)), the contact area reduces to an almost line contact from a rectangular contact at 5.17° of flexion (see Figure 4.21(b)). The smaller contact area in combination with large tibiofemoral contact forces results in high contact pressures, such as the 56MPa seen in the UHMWPE inlay at 130°. Generally, the higher the contact pressure, the higher the probability of abrasive wear [118].

The compliancy of the PCU inlay results in greater deformation compared to UHMWPE, which in turn will increase the effective contact area and therefore a decrease in contact pressure and potentially a decrease in the risk of wear. This was observed in the results presented in this thesis (see Table 4.3).

The discussion of a few specific results that have been observed in the PCU tibial inlay simulations will now be presented.

**Specific Observations of the Performance of the PCU Inlay**

Analyzing the simulation results of the squatting load scenario have revealed a possible limitation for the use of compliant polymers in TKRs. In the natural knee at high flexion angles, such as during squatting, the femoral component moves to the posterior edge of the tibial inlay. This effect is called femoral rollback. In the FE knee model employed in this thesis, the femoral rollback was simulated by anteriorly translating the tibial inlay. Due to the low stiffness of the PCU tibial inlay and the posterior position of the femoral component, the simulation predicted large deformation in the tibial inlay. The posterior wall of the inlay extends outwards and it appears that the inlay is pushed posteriorly (to the left of the picture of the inlay model shown in Figure 4.23). It is believed that the fixation of the inlay within the tibial tray is the main reason for this bulging. The substrate is rigidly fixed to the tibial tray (simulating a fixed attachment of the inlay to the tibial inlay).
and the bottom of the substrate can therefore not move, hence the bulging. Because of
the axial force that is applied while the tibial inlay is translated anteriorly and the friction
between the inlay and the femoral component, the articular surface of the inlay “sticks”
to some extent to the femoral component which does not move. The higher the frictional
force, the more “sticking” would occur. The “sticking” together with the axial force and
the constraint substrate bottom, cause the posterior bulging of the tibial inlay. In a real
TKR, it is possible that the tibial inlay may be pushed out of the tibial tray. The inlay may
have to be redesigned when using a PCU inlay in such a way that the fixation mechanism
can withstand any occurring AP or ML forces. This might require a novel design of inlay
fixation, completely different to that currently used with UHMWPE.

As observed in Figure 4.24 in Section 4.3.1, there may be an impingement issue of the
femoral shaft against the tibial inlay at flexion angles of 130° and higher. The issue of
impingement of the femoral shaft against the tibial inlay has been observed in a fluoroscopy
study of a deep squatting exercise [15]. The group reported a mean maximum knee flexion
angle of 117-121.7° depending on the measurement method. Figure 5.1 shows an example
of such a fluoroscopy image at deep flexion where impingement occurs (as highlighted in
this figure). It is possible that the flexion angle investigated in this thesis is higher than
the angle at which impingement occurs for the TKR modelled in this thesis. However, the
TKR used in this thesis has been designed to account for high-flexion angles of up to 155°
and the 130° tested in this thesis, should therefore not be an issue. It is more likely that
the position of the femur with respect to the inlay in this thesis is different to the actual in
vivo position of the femur in squatting. If the TKR forced the femur into a more posterior
position during high flexion, impingement might no longer occur.

This section has discussed the findings from the FE knee model simulations using App-
proach I. Now, The findings from the FE knee model simulations using Approach II will be
discussed.
Figure 5.1: Fluoroscopy image of a TKR in deep flexion. An area of possible impingement of the posterior side of the tibial inlay against the femur is shown, reproduced from Bellemans et al. [15]
5.3.2 FE Knee Model Simulations using Approach II

In order to assess the performance of a compliant tibial inlay over a wide range of continuous flexion angles instead of only a few discrete angles, a dynamic gait cycle simulation was attempted using the original knee model (see Section 3.3.3 for a description of Approach II).

In Section 4.3.2, it was shown that using the original, explicit FE knee model could not be used with PCU. This is believed to be due to the pressure overclosure function utilized (see equation (3.9)), which has been developed for compressible materials. The application with incompressible materials, such as PCU, leads to numerical problems (division by 0), unless the Poisson’s ratio is adjusted. However, assuming $\nu$ to be 0.495 in the pressure overclosure function (see Section 3.3.1), results in very high contact pressures, even at small deformations. The pressure in the pressure overclosure function in simulations with rigid bodies has a similar function as the elastic modulus in simulations with deformable bodies. The high pressure values are therefore thought to be responsible for the lack of deformation occurring in the PCU tibial inlay. The rigid FE knee model using the pressure overclosure function overestimates the stiffness of the polymer. Lowering the Poisson’s ratio to values used in fully compressible materials ($\nu \leq 0.46$) resulted in increased tibial inlay deformation, showing that using a $\nu$ close to 0.5 is the main reason to explain why Approach II was not successful.

It can be concluded that Approach II does not work for incompressible materials in general. Unfortunately, it was not possible within the scope of this thesis to find a pressure overclosure function for incompressible materials that could be used in the Abaqus contact definition.

Explicit Simulation with a Deformable Inlay

In addition to the explicit simulation using a rigid inlay, a simulation using the explicit FE knee model with a deformable inlay was also attempted. This would allow the assessment of
the compliant tibial inlay over a continuous range of flexion angles with only one simulation. A major issue with running deformable explicit simulation is that it is very time-consuming, due to the very small time-increments required to achieve a converging solution. It is often possible to increase the increment size by increasing the density of the material. However, increasing the density can lead to less realistic results depending on how much the density is changed, since this influences the dynamics of the model. Both global (manual) and local (automatic) mass-scaling (change of density) was employed, resulting in a decrease in computational time. The inlay was unrealistically deformed in this model and contact was being established where there should not be any. Therefore, these results were discarded.

Using a UHMWPE inlay that has a significantly higher elastic modulus than PCU (roughly 30 times higher) resulted in more realistic simulation results. It is believed that the mass scaling in combination with the very low elastic modulus of PCU was the major source of error, since mass-scaling in the UHMWPE inlay yielded reasonable results. The exact reasons for the contact issues could not be determined, as the same contact definition worked with UHMWPE. However, the contact issues could also be a result of the low elastic modulus and mass-scaling.

5.4 Limitations of the Model Used in Approach I

In this FE analysis of a compliant polymer inlay of a TKR, only static discrete loading conditions were considered and therefore a nonlinear elasticity material model was used. However, the human knee joint is subject to millions of cycles of varying loads (the velocity at which these loads are applied also varies), which could not be taken into account in this project. It has been shown that PCU exhibits time-dependent deformation behaviour (see Section 4.1.1), which would most likely play a major role in the performance of the TKR in loading scenarios occurring in the natural knee. Nevertheless, as observed in Section 4.1.1, the stress relaxation, and therefore also the creep, is a finite process and an equilibrium
state may be achieved after a certain amount of time. So, while the geometry of the
inlay and therefore the kinematics of the TKR will change over time, the changes may not
be too significant. This may benefit from further investigations. It was shown that PCU
exhibits hysteresis upon unloading and this is likely to occur during cyclic loadings in the
knee, but this hysteresis was not considered in the static loading approach chosen in this
project.

The validation of the Yeoh material model has shown that the deformation behaviour
when motion is constraint is not accurately simulated. This could influence the stress and
strain results of the tibial inlay in the region close to where it is fixed to the tibial tray.
However, it has been shown that the material model overestimates stress, so the results
presented here can be considered to be a worst case scenario.

In Approach I, only axial tibiofemoral loads are applied to the knee model. However,
gait analysis has clearly shown that other forces and moments are also present, such as AP
force and abduction/adduction moments. The tibiofemoral contact force is, however, the
largest force acting on the knee and it has therefore been considered valid to exclude other
forces in this project. Also, the only DOF considered in this thesis, is flexion of the knee
joint. The femoral component was brought into its rotated position without considering
any other movements. While the tibial inlay was allowed to move freely during flexion,
this might not represent the actual motion that occurs in reality. Other rotations, such as
abduction/adduction and internal/external rotation, which have been shown to occur, were
not considered and could influence the outcome of the simulations. The FE knee model
employed in Approach I also does not include effects due to soft tissue.
Chapter 6

Conclusion

In order to assess the performance of compliant polymers in TKR using FEA, two different polycarbonate urethanes (PCUs), PCU55D and PCU80A, were mechanically characterized. The obtained test data was used to determine material specific coefficients of the hyperelastic Yeoh model. The Yeoh model was then used in an FE knee model, which was developed and adjusted so that the deformation, von Mises stresses, contact areas and contact pressures, occurring in a compliant PCU tibial inlay of a TKR during some typical knee loadings, could be investigated. The von Mises stresses, contact areas and contact pressures found in the PCU inlay were compared to literature and a UHMWPE tibial inlay.

6.1 Important Findings from the Mechanical Experiments

Several stress-strain characteristics were observed in the mechanical test data, which are typical for elastomers:

- Test results were generally found to be repeatable.
- It was found that the compressive deformation behaviours of PCU55D and PCU80A show similar features. Hysteresis during unloading was observed and under cyclic
loading, residual strain and stabilizing deformation behaviour after six to seven cycles were observed that reoccur whenever the maximum strain is increased. This is typical for a material subject to softening. However, the typically reported difference between the first stress-strain curve and subsequent stress-strain curves, in which the subsequent stress-strain curves are much more compliant, was not observed.

- No significant relationship between strain rate and mechanical behaviour for PCU55D or PCU80A was detected.

- The cyclic stress relaxation experiments revealed similar behaviour to cyclic uniaxial compression experiments, with the addition of stress relaxation. The relaxation was found to be nonlinear, indicating that the amount of stress relaxation depends on the strain level.

- Constrained plane strain compression experiments revealed the same features (residual strain, stabilization etc) found in the equivalent unconstrained tests. However, constraining one lateral movement resulted in a stiffer stress-strain response.

6.2 Important Findings from the FE Material Behaviour Modelling

Using the stabilized loading curve of the cyclic unconstrained compression test data, the hyperelastic Yeoh material model was tuned and validated using cyclic unconstrained compression test data and plane strain experimental data. The following points were noted:

- The Yeoh material model yielded good curve fits of all stabilized test data. Some deviation between curve fits and test data occurred for strains less than 0.25. As observed in the experimental test data, the curve fit results did not reveal any clear strain-rate dependency either. To account for the variability in the test data, lower bound, overall mean and upper bound Yeoh coefficients were calculated from all curve
fit results. It was concluded that the Yeoh material model is appropriate for the experimental data obtained in this project.

- Validation of the plane strain results showed poor agreement with experimental data. The accuracy below strains of 0.2, however, is acceptable. It may be necessary to conduct multi-axial experiments in addition to uniaxial experiments to obtain better Yeoh material coefficients capable of predicting constrained compression behaviour. Using quadratic elements may also improve the predictions of constrained compression.

### 6.3 Important Findings from the FE Knee Model Simulations

It follows a list of the major findings of the FE knee model simulations:

- For both PCU and UHMWPE, the simulated contact area between the tibial inlay and the femoral component decreases and the simulated contact pressure in the tibial inlay increases with increasing knee flexion angle.

- Simulated UHMWPE tibial inlay peak contact values for angles greater than 15° may exceed the compressive yield strength of UHMWPE, indicating that there may be an increased risk of wear.

- Simulated UHMWPE tibial peak contact pressures and contact areas between the UHMWPE tibial inlay and the femoral component found in this project compare well with literature, indicating that Approach I (see Section 4.3.1) is valid.

- Simulated PCU tibial inlay contact pressures are up to 82% lower than values observed in the UHMWPE tibial inlay. PCU contact areas in the simulation are up to 437% (at 130° of flexion) larger than simulated UHMWPE tibial inlay contact areas.
• Contact pressures of the tibial inlays when modelled in the simulation with PCU are well below the maximum stress values reached in the mechanical experiments reported in this study. Since these values did not seem to result in permanent damage, it is believed that the contact pressures observed in the simulations which use PCU as the inlay material are lower than the compressive yield strength of PCU, therefore potentially minimizing the risk of wear.

• Large deformation and bulging of the posterior wall of the PCU inlay at high flexion was observed in the simulation and possible slipping of the tibial inlay out of the tibial tray fixation might necessitate redesigning the inlay to ensure adequate fixation.

• PCU contact areas approach values reported in literature for the natural knee, indicating that the a TKR with a PCU inlay is a first step towards a more cartilage-like knee joint.

• Using a static FE knee model to simulate discrete knee loading scenarios, the performance of the PCU tibial inlay was found to be favourable, and the compliant nature of PCU may provide unique advantages over a UHMWPE tibial inlay by exhibiting very low contact pressures and higher contact areas between the tibial inlay and the femoral component which is thought to more closely mimic the behaviour of the natural knee. Initially less congruent knee designs which deform on loading to increase contact area, and possess a greater range of motion might therefore be feasible. It was shown that PCU has the potential to be a successful component in the tibial component of a TKR.

• The FE simulation results indicated that, for the loading conditions investigated in this report, a double layer PCU tibial inlay consisting of a PCU55D substrate and a PCU80 articulating layer is feasible for a TKR.
6.4 Possible Future Work

During researching this project, many avenues of investigation were identified, but the limited scope of this thesis meant that not all of these could be considered. These other research areas together with specific questions raised by this research project, identify topics which may be valuable to address in future work. A summary of ideas for future work is now described.

6.4.1 Mechanical Testing

- Compression testing at a greater range of strain rates in cyclic testing may detect the presence of strain rate dependency.
- Compression testing at at least one additional temperature, for example room temperature, may reveal whether temperature influences the strain rate dependency and the amount of softening.
- Shear and biaxial compression testing may help to improve the performance of the hyperelasticity model so that it more accurately predicts multiaxial stress states.

6.4.2 FE Material Behaviour Modelling

- The investigation of a more detailed data set to derive material coefficients and the use of quadratic elements may improve the hyperelasticity model.
- The inclusion of time-dependency, hysteresis and softening in the FE material modelling may improve the simulation of a dynamic load case, such as a gait cycle. This may be achieved by either using Abaqus built-in material models, such as viscoelasticity (Prony Series), hysteresis option for hyperelasticity or the Mullins effect, or by using the capability of Abaqus to code a more advanced material model, such as the Qi-Boyce model for PUs [11] or the general elastomer model by Bergstroem and Boyce.
[157, 158], using a user material subroutine (UMAT) that requires writing a code in FORTRAN.

6.4.3 FE Knee Model Simulations

- The simulation of more complete loading including internal/external rotation and anterior/posterior displacement may more closely resemble normal physiological gait situation.

- The long term performance of the PCU inlay using Approach II (see Section 3.3.3) maybe be further developed to simulate continuous loading scenarios, by either using the original explicit FE knee model with a deformable inlay or building up on the combined explicit and implicit modeling approach described in this thesis.

- The simulation of different designs may be performed to investigate the influence of geometry on the performance of the PCU tibial inlay. Also, more functionally graded inlays could be investigated that use a compliant layer only where required, with layer thickness defined by expected loadings. This may help to further improve the TKR and obtain a solution that is even closer to the natural knee.

- The work presented in this thesis could be expanded to other joints, because findings from this project are likely to be applicable to other joints such as the hip.
Chapter 7

Summary

The aim of this study was to assess the feasibility of using a compliant polymer in a TKR application using FEA. A two layer tibial inlay consisting of a stiff PCU55D substrate and a more compliant PCU80A articulation layer was investigated for a TKR. Mechanical test data from compression experiments was used to tune a hyperelastic material model which was then applied to a FE knee model, in which five different static loading scenarios, three gait cycle events, stair climbing and squatting, were simulated. The performance of the compliant PCU inlay was compared to literature and to a standard UHMWPE inlay.

The mechanical test data has shown that PCU55D and PCU80A exhibit typical elastomeric deformation behaviour, such as stiffening at higher strains, stabilized deformation behaviour after six to seven cycles and time-dependency.

Validation of a Yeoh hyperelastic material model tuned with test data has shown good results for unconstrained test data, but revealed that further investigations may be necessary to improve the accuracy of estimating multi-axial test data.

The differences of the contact area and peak contact pressure of tibial inlays modelled with UHMWPE and PCU were quantified and showed that the simulated contact area for a tibial inlay modelled with PCU was on average 345% greater than the contact area of a tibial inlay modelled with UHMWPE and close to what has been reported for the natural knee.
The simulated contact pressure was on average 77\% lower in tibial inlays modelled with PCU than in tibial inlays modelled with UHMWPE. Contact pressures simulated for tibial inlays modelled with PCU were below values that may cause damage, possibly minimizing the risk of wear.

The fact that the contact pressures were low even at high flexion angles, when congruency is very limited, suggests that an initially less congruent knee design that still exhibits low contact pressures, might be feasible and allow for a greater range of motion. The findings of this thesis strongly indicate that compliant polymers may be feasible for use in a TKR application as a tibial inlay, in an effort to develop a TKR which more closely mimics the natural knee.
Bibliography


Appendix A

FE Material Behaviour Modelling

A.1 Hyperelasticity Curve Fit Results

In Section 4.2.1, only the mean Yeoh coefficients with standard deviation for each test condition (see Table 4.1) and overall mean values of all test conditions (see Table 4.2) were reported. For completeness, all the individual Yeoh coefficients for each test condition are listed in Table A.1.
Table A.1: Curve fit results of Test 1 - Complete set of Yeoh coefficients

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† Tested in Winterthur, ‡ Tested in Warsaw
Appendix B

FE Knee Model Simulations

B.1 Coordinate Systems

As described in section 3.3.1, two different coordinate systems (CSs) were used per bone or TKR component, totalling in four CSs. There are two anatomical CSs, which are defined using anatomical landmarks, and are hereafter referred to as JEF CSs. The second set of CSs, which will be referred to as ISO CSs, are in accordance with the ISO definition [14]. A description of the four CSs now follows [149].

B.1.1 JEF Coordinate System (Anatomical)

The JEF CSs were defined using a custom-made Matlab (Mathworks, Natick, MA, USA) program. The JEF CS of the femur is defined as followed. The y-axis, which points proximally (towards the hip), is defined as the normal vector of a plane tangentially fitted to the most distal femoral surface and is approximately parallel to the mechanical axis of the femur. The x-axis points anteriorly and is the normal vector of a plane that is tangential to the most posterior femoral surface. The z-axis, is defined as the cross product of the other two axes and points medially. The origin of the femoral JEF CS is situated between the femoral condyles.
The direction of the z-axis of the tibial JEF CS is identical to the one of the femoral JEF CS. The normal of the tibial plateau rotated about the z-axis by $6^\circ$ and about the x-axis by $3^\circ$ to account for the posterior slope and medial slope, respectively, is defined as the y-axis. Lastly, the x-axis is the cross product of the y- and z-axes. The origin of the tibial JEF CS is defined on the plateau as the cross point of the ML and AP dimension.

B.1.2 ISO Coordinate System

The flexion axis is defined in the following manner according to the ISO standard: Two imaginary planes perpendicular to the tibial axis are considered, one at $30^\circ$ flexion and one at $60^\circ$ of flexion of the femoral component. The medial and lateral condyles of the femoral component would contact the two planes in four different points (two points at each flexion angle) and from these points four contact normals, perpendicular to the imaginary planes, can be visualized. The line that intersects all four normals is considered to be the flexion axis.

Because the two normals of each imaginary plane are parallel, two new planes can be built. The intersection of the two planes is the ISO CS x-axis (flexion or ML-axis) of the femur. The direction of the z-axis (proximal/distal) is identical to the direction of the anatomical y-axis (JEF CS). Taking the cross-product of the x- and z-axes yields the ISO CS y-axis of the femur. The origin of the ISO CS of the femur is defined as the intersection of the ISO x-axis and the anatomical femur x-y-plane of the JEF CS.

A description of the tibial ISO CS now follows. The axial force axis of the ISO gait cycle is parallel to the tibial long axis with a $0.07 \times w$ (w is equal to tibial inlay width) medial offset and is pointing proximally (cranially) [14]. The long axis is assumed to be equal to the direction of the JEF CS y-axis (mechanical axis of tibia). To create the ISO CS z-axis (proximal/distal), a plane perpendicular to the JEF CS y-axis of the tibia and close to the distal end of the modeled tibia is built. The position of the ISO CS z-axis is defined as the
midpoint of all tibial vertices intersecting the constructed plane. This point approximates
the centre of the medullary cavity. The projection of this point along the ISO CS z-axis
of the tibia onto the x-z-plane of the tibial JEF CS yields the origin of the ISO tibia CS.
The ISO tibial torque axis [14] is also equal to the ISO CS z-axis and points proximally
[149]. The ISO CS y-axis (anterior/posterior), is, in accordance with the ISO standard,
perpendicular to the tibial ISO CS z-axis and the femoral ISO CS x-axis (medial/lateral)
and therefore points anteriorly.

The JEF and ISO CSs for the tibial inlay and femoral component are presented in
Figure B.1.
B.2 Simulation Results

In Section 4.3.1, the contact pressures in the PCU and UHMWPE tibial inlay were compared for 5.17° of knee flexion and 130° of knee flexion. These two cases represented the smallest and largest flexion angle investigated. However, as described in Section 3.3.2, other flexion angles were also investigated. The simulated contact pressures for a flexion angle of 10.15°, 15.83° and 56.6° are shown in Figure B.2.

Comparing the PCU tibial inlay contact pressures (left column in Figure B.2) with the UHMWPE tibial inlay contact pressures (right column in Figure B.2), substantiates the findings from Chapter 4.3.1, where it was shown that the contact pressure in PCU is significantly lower than in UHMWPE. Also, as observed before, the contact pressure in the tibial articular surface is an indicator of the contact area between the tibial inlay and the femoral component. The area with contact pressure clearly indicates that the contact area in the UHMWPE inlay is significantly smaller than in the PCU inlay.
APPENDIX B. FE KNEE MODEL SIMULATIONS

Figure B.2: Comparison of contact pressure between PCU and UHMWPE inlay for 10.15°, 15.83° and 56.6° flexion. Scales are not consistent in all figures to more accurately illustrate the complete contact pressure distribution.