A HYBRID AI–PHYSICS FRAMEWORK FOR SYNTHETIC BIOMECHANICAL MODELLING AND WEAR PREDICTION IN MODULAR ALL-POLYMER KNEE TRAYS (PEEK-OPTIMA™)

A Digital Transformation Approach in Orthopaedic Data Science

Obasi Chinedu Chamberlin

Supervisor:
Dr. Mitha Rachel Jose, Senior Lecturer, Laurea University of Applied Sciences

Date: 28.02.2026

Co-funded by the European Union

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Dedication

According to Ecclesiastes 9:11, the race is not to the swift, nor the battle to the strong but time and chance happen to them all.

This academic journey has been shaped by the support, sacrifices, and encouragement of many people, who contributed in different ways to make it meaningful. Some of these individuals are no longer here to witness the outcome of their efforts, especially my beloved mother, whose absence leaves a void that can never truly be filled.

In gratitude and remembrance, I humbly dedicate this thesis to the cherished memories of:

My Late Mother:
Lolo Obasi Florence Obiageri

My Late Mentors:
Engr. Everest Nwosu
Nze Ignatius M. D. Umunnah
Dr. Alamba Chukwuma Samuel

Your sacrifices and guidance laid the foundation upon which I continue to build today.

May the peace of God be with you until we meet again.

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provided the benchmarks against which my work could be evaluated. I hope this thesis contributes, in some small way, to the body of knowledge they have built.

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Abstract

Digital transformation in healthcare increasingly integrates artificial intelligence (AI), and computational modelling, to complement traditional experimental validation of medical devices. Total knee replacement (TKR) implants, require extensive mechanical, and tribological evaluation, which remains time-intensive and resource-demanding. This study developed and validated a quantitative, physics-informed, data-driven digital framework for generating synthetic biomechanical data and predicting stress, deformation, and wear behaviour in modular all-polymer knee trays manufactured from PEEK-OPTIMA™.

A synthetic dataset, comprising 8000 design configurations, was generated using Latin Hypercube Sampling, across literature-supported geometric, material, and loading ranges. Stress and deformation, were estimated using simplified contact mechanics relationships, while wear was modelled using Archard's wear law. Supervised regression models, including Random Forest, Gradient Boosting, and Artificial Neural Networks, were trained to predict biomechanical responses. Ensemble tree-based models achieved high predictive accuracy for stress ($R^2 > 0.98$) and deformation ($R^2 \approx 0.95$). Wear prediction demonstrated moderate explanatory power ($R^2 \approx 0.59$), reflecting the nonlinear and cumulative nature of tribological processes.

Validation against ISO 14243 loading standards and multi-design OrthoLoad in vivo envelopes confirmed physiological plausibility. The framework demonstrated that physics-informed synthetic data, combined with machine learning, can support early-stage digital screening of implant designs.

Keywords: PEEK-OPTIMA™, Total Knee Replacement, Synthetic Biomechanical data, Biomechanical Modelling, Machine learning, Digital Transformation in healthcare

JEL Classification Codes: C45, I19

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Glossary

Term / Acronym	Meaning
AI	Artificial Intelligence
ANN	Artificial Neural Network
Archard's Law	A physics-based wear equation that relates wear volume to applied load, sliding distance, hardness and a wear coefficient.
EDA	Exploratory Data Analysis
FAIR Principles	Data management principles ensuring that data are Findable, Accessible, Interoperable, and Reusable
FEA	Finite Element Analysis
GB	Gradient Boosting
GBM	Gradient Boosting Machines
GDPR	General Data Protection Regulation
ISO	International Organization for Standardization
ISO 14243	International standard specifying wear testing procedures for knee prostheses
LHS	Latin Hypercube Sampling
MAE	Mean Absolute Error
ML	Machine Learning
MLP	Multilayer Perceptron
MPa	Megapascal, a unit of stress
OrthoLoad	Database containing in-vivo joint load measurements from instrumented orthopaedic implants
PEEK	Polyetheretherketone, a high-performance thermoplastic polymer
PEEK-OPTIMA™	Medical-grade PEEK polymer commonly used in orthopaedic implants
RMSE	Root Mean Square Error
RF	Random Forest
R^2	Coefficient of Determination (measure of model predictive accuracy)

Term / Acronym	Meaning
TKR	Total Knee Replacement
Wear Rate	The rate of material loss during contact and sliding between surfaces

Introduction

This thesis investigated the application of data-driven modelling approaches, to simulate biomechanical behaviour, and wear prediction in modular all-polymer knee implant components manufactured from PEEK-OPTIMA™. Advances in artificial intelligence and computational modelling, have created opportunities, to support orthopaedic device development, through digital experimentation, reducing reliance on time-consuming, and costly physical testing procedures.

Total knee replacement (TKR) implants, are traditionally validated using experimental wear simulators, and finite element modelling. While these methods provide valuable insight, they often require extensive resources, and may limit rapid design exploration. Emerging data science approaches, such as, the use of synthetic data, offer an alternative pathway, by enabling predictive modelling of biomechanical responses under simulated physiological conditions.

In this study, a synthetic biomechanical dataset, was generated using Latin Hypercube Sampling, to represent realistic combinations of implant design parameters, and loading conditions. Machine learning models were then developed, to predict stress and deformation responses, and these predictions were integrated with Archard's wear equation, to estimate potential wear behaviour.

The research contributes to the growing field of digital orthopaedics, by demonstrating a hybrid physics-informed and machine learning framework, capable of approximating biomechanical responses relevant to implant performance assessment.

Chapter 1
Background and Research context

1.1 Background and Context

Following the incident of corona virus, a new era has been ushered in. This new era called digital transformation, characterised by strategic adoption of digital technologies, has changed mankind for ever; by changing the way we live, work and learn. No aspect of modern life is left behind.

It has altered healthcare systems progressively (Obasi & Banigo, 2026; Topol, 2019), by the integration of digital technologies, such as , computational modelling (Viceconti et al., 2016), artificial intelligence (AI)(Kazeminia et al., 2019) , and synthetic data into clinical and biomedical research processes (Chen et al., 2021; Kokosi & Harron, 2022; Reich et al., 2025; Viceconti et al., 2016). In the development of orthopaedic devices, this shift presents opportunities to expedite design processes (Fu et al., 2025), reduce experimental expenses and duration, and enhance consistency in biomechanical evaluations (Donnelley et al., 2021).

In orthopaedics, total knee replacement (TKR) appears to be one of the most significant surgical procedures, that are carried out globally for the treatment of musculoskeletal injuries and degenerative diseases, restoring function and reducing pain (Misir, 2025). However, these implants must have adequate mechanical integrity, and wear performance for them to last long after their implantation, and reduce post operation revision. (Misir, 2025). The tibial tray which is a major component of the implant, performs a vital structural role during usage by distributing joint loads, while remaining stable under repeated cyclic loading (Mueller et al., 2025).

To evaluate prosthesis durability under gait-like loading conditions, standardised mechanical testing methods detailed in ISO 14243-1 and ISO 14243-3, are used to provide the required controlled wear simulation protocols (ISO *14243-1*, 2009; ISO *14243-3*, 2014). On the other hand , in-vivo joint forces gathered from instrumented implants, and stored in OrthoLoad database, are used to deliver essential insights into physiological loading levels and patterns during daily activities (Bergmann et al., 2014).

Previously, orthopaedic knee implants components were made from mostly metal alloys, such as, titanium alloys and cobalt-chrome, given their superior mechanical strength, durability and biocompatibility (Marin & Lanzutti, 2023). However, they are associated with stress shielding, the release of wear debris and metal ions , leading to implant loosening and prevention of imaging, especially, postoperatively (Lodge et al., 2023). On the other hand, polymeric biomaterials have received much attention, due to their suitability to address some of these challenges posed by these metal alloys (Lodge et al., 2023).

PEEK-OPTIMA™, a medical-grade polyetheretherketone (PEEK), has surfaced as a suitable replacement for standard metal-backed tibial components, thanks to its bone-like rigidity, radiolucency, and biocompatibility (Kurtz & Devine, 2007). Nonetheless, its biomechanical response and wear characteristics under repeated loading should be assessed thoroughly.

Given the recent developments in machine learning, we can now model the complex biomechanical systems, without extensive simulation (Karniadakis et al., 2021). Synthetic data generation techniques, on the other hand, have further allowed us to explore multidimensional design spaces. This convergence, however, now drives the creation of physics-informed digital assessment frameworks for evaluating orthopaedic knee implants.

1.2 Problem Statement

In computational biomechanics, despite the advances that have been recorded already, current implant validation remains dependent on:

- High computational cost of FEA.
- Limited access to experimental wear simulators.
- Data scarcity and proprietary restrictions.
- Ethical considerations in human data usage.

There is a need for scalable, reproducible, and computationally efficient digital methods that can estimate biomechanical trends in the early-stage of implant design.

1.3 Research Aim and Objectives

1.3.1 Research Aim

The primary aim of this study was to develop and validate a quantitative, physics-informed, data-driven digital framework that can be used to generate synthetic biomechanical data and predict stress, deformation, and wear behaviour in modular all-polymer knee trays manufactured from PEEK-OPTIMA™, in-order to support early-stage digital evaluation, in orthopaedic device development.

1.3.2 Objectives

1. To develop a synthetic data generation pipeline using Latin Hypercube Sampling.

2. To train and evaluate machine learning models for stress and deformation prediction.

3. To integrate Archard's wear equation into a hybrid digital framework.

4. To validate predicted loading ranges against ISO 14243 and OrthoLoad datasets.

5. To ensure transparency and reproducibility aligned with FAIR data principles.

1.4 Research Questions

1. Can synthetic data generation combined with physics-informed modelling predict biomechanical trends in modular all- polymer PEEK-OPTIMA™ based knee implants?

2. Which regression models perform best for structured biomechanical datasets?

3. Can hybrid AI-physics approaches produce physiologically realistic wear estimates?

1.5 Scope and Limitations

This research is focused on digital simulation and trend-based mechanical evaluation rather than clinical outcome prediction. As a result the following limitations exist:

- Stress and deformation proxies were estimated using simplified mechanical relationships rather than detailed finite element simulations.

- The wear model is based on Archard's equation and does not include complex time-dependent material effects.
- Clinical validation and experimental wear testing are outside the scope of this study.
- Experimental calibration and patient-specific modelling are beyond the scope of this work.
- Waveform replication of ISO simulators is outside the present scope.

The framework is intended, for early-stage digital screening, rather than regulatory or clinical certification.

1.6 Significance and Expected Contributions

This study is meant to contribute to digital orthopaedics in the following ways:

- Demonstrating feasibility of physics-informed synthetic modelling.
- Comparing ensemble and neural regression approaches.
- Providing a reproducible computational workflow.
- Supporting early-stage implant screening.

1.7 Thesis Structure Overview

The general structure of this thesis is arranged into five (5) chapters after the introduction page. The background and research context started the chapters, followed by the review of relevant literature, then, methodology, to results, discussion, and finally, conclusion.

The Chapter 1, introduced the research context, the problem statement, and the study objectives. It clearly outlined the motivation behind the development and validation of a digital, physics-informed framework for predicting biomechanical behaviour and wear in modular all-polymer PEEK-OPTIMA™ knee trays.

The Chapter 2, searched the relevant literature on knee joint biomechanics, implant design considerations, wear modelling approaches, and the application of artificial intelligence in biomechanical engineering. The chapter also, streamlined the search from anatomical function of the knee, mechanical foundations to computational modelling methods and identified the research gap that this study addressed.

Then, in Chapter 3, the methodology used in the study was introduced. It described how the synthetic data was generated using Latin Hypercube Sampling method, the formulation and application of the simplified mechanical relationships that were used for stress and deformation prediction, the implementation of machine learning regression models, and the integration of Archard's wear equation, within a hybrid modelling framework. Validation approaches and reproducibility considerations, were described thoroughly in the study.

The chapter 4, reported the results of the synthetic dataset analysis, the performance of the models evaluation, the wear calculations, and the validation benchmarking against ISO standards and in vivo loading datasets. The statistical metrics and sensitivity analyses used to assess the robustness and biomechanical realism of the models were presented.

The Chapter 5, discussed the results of the study and the implications of the findings in the light of existing literature. It also, evaluated the strengths and limitations of the proposed framework as well as the methodological assumptions. In addition, the potential future developments of the study in digital orthopaedic engineering was outlined.

Finally, the thesis concluded by summarising the key findings, evaluating the achievement of research objectives, and highlighting the contributions, the study made to digital transformation in orthopaedic implant design.

1.8 Disclosure of AI Use

During the development of this thesis, artificial intelligence tools were used as research assistants to support the author's original work. Specifically:

- ChatGPT was used for brainstorming ideas, and obtaining guidance on complex technical concepts, while QuillBot was used for language polishing, plagiarism and AI checking.

- AI-generated templates were offered as learning aids; and such contents were later adapted by the author in his own words, and all sources cited were independently located and verified by the author.

Chapter 2
Literature Review

2.1 Orthopaedic Implants and Total Knee Replacement

To undertake a literature review of this type, one has to be extensive, diverse and interdisciplinary. As the topic centres on orthopaedic biomechanics, total knee replacement (TKR), polymer implant materials, tribology, machine learning and synthetic data generation.

To understand the mechanical behaviour of knee implants, one has to combine knowledge from anatomy, materials science, computational modelling, artificial intelligence (AI), and clinical device evaluation (Rocha et al., 2025). This chapter synthesised diverse academic domains to establish the context of the present study, which focuses on a digital, physics-informed, data-driven framework for predicting biomechanical behaviour and wear in modular all-polymer PEEK-OPTIMA™ knee trays.

2.1.1 Functional Anatomy of the Knee Joint

The knee is one of the marvels of life´s movements system. A proper description of its inner working is beyond the scope of the thesis. However, to understand how the artificial implant works, a clarification of the functional elements of the knee is necessary.

The knee is our body's largest, most complex load-bearing synovial hinge joint, that mainly enables flexion (bending) and extension (straightening), and carries out an important role in the movement , and stability of our body (Rocha et al., 2025).

Functionally, as a connector, the knee joint is stabilised by four main ligaments that join the femur (thigh bone) to the tibia (shin bone) and fibula; cushioned by menisci, and lubricated by synovial fluid , all essential for controlling motion and preventing injury (Masouros et al., 2010). For more details, the knee has 4 main ligaments:

- Medial collateral ligament (MCL*)*: on the inside of the knee near the midline.
- Lateral collateral ligament (LCL): on the outside of the knee.
- Anterior cruciate ligament (ACL): inside of the knee and crosses to the front.
- Posterior cruciate ligament (PCL): inside of the knee and crosses to the back.

The two cruciate ligaments (ACL, PCL) are for back-and-forth stability while the other two collateral ligaments (MCL, LCL) are for side-to-side stability. Figure 2.1 depicts the functional anatomy of the human knee joint with its relevant anatomical parts necessary for its function.

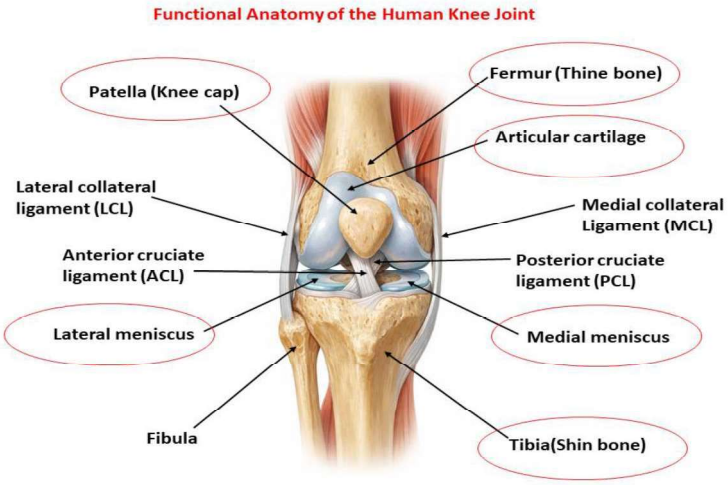


Figure 2.1. Schematic representation of the human knee joint illustrating primary load bearing structures. Source: Adapted from an AI-generated image produced using ChatGPT (OpenAI, 2026).

With regards to structure, the knee comprises three main articulations: the medial tibiofemoral joint, the lateral tibiofemoral joint, and the patellofemoral joint (Escamilla et al., 2012; Nordin & Frankel, 2012). In a normal knee, these articulations are responsible for an organised load transfer between the femur and tibia and facilitate locomotion across diverse activities of daily living.(Nordin & Frankel, 2012).

2.1.2 Biomechanics of the Knee joint and Tibial Tray function

In general , the choice for artificial knee implant, whether partial or total knee replacement is based on the nature of the knee joint wear, its position and features (Slullitel et al., 2024). Total knee replacement (TKR), entails substituting the complete knee joint, including the femoral and tibial surfaces, with anatomically designed artificial parts aiming to restore normal joint function and allow a full range of knee flexion (Slullitel et al., 2024). Accordingly, the surgeon has the duty to select the most suitable artificial knee implant design for each patient.

In a normal total knee replacement (TKR) system, the following components are common:

- the femoral component
- the tibial tray
- the polyethylene insert , and
- the patellar component (optional), as shown in figure 2.2.

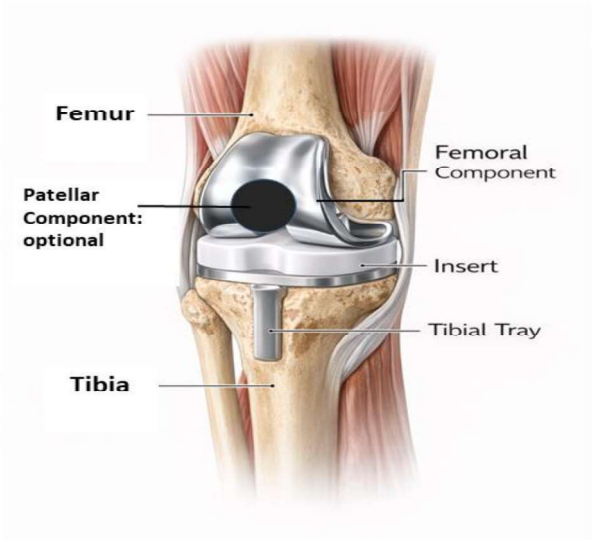


Figure 2.2. Schematic representation of Total Knee Replacement: the human knee joint with implanted Artificial Knee Implant. Source: Adapted from an AI-generated image produced using ChatGPT (OpenAI, 2026).

During normal gait, the knee undergoes cyclic flexion and extension while sending significant compressive and shear forces between the femur and tibia. In a study using instrumented implant, it was showed that axial joint forces during walking may exceed two to three times body weight (Bergmann et al., 2014).

To support polyethylene as a bearing surface, the tibial tray must perform a critical structural duty by sharing the load from the femoral component to the tibial plateau (Mueller et al., 2025). Otherwise, the excessive contact stress or uneven load distribution, may contribute to implant loosening (Nordin & Frankel, 2012), polyethylene wear (De Ruiter et al., 2017), and long-term failure (Bartel et al., 1986). Consequently, a good knowledge of this load transfer mechanism is essential when evaluating stress distribution, deformation behaviour, and long-term wear performance of tibial tray designs (Bartel et al., 1986; Bergmann et al., 2014).

The mechanical performance of the tibial components depends on many related variables, such as , the geometry, material stiffness, conformity, and loading magnitude (Bartel et al., 1986; Mueller et al., 2025). Classical contact mechanics principles, indicate that stress is directly proportional to applied load , and inversely proportional to contact area, while deformation is influenced by elastic modulus and component thickness (Korkusuz, 2016; Nordin & Frankel, 2012). In basic digital modelling approaches, these first order mechanical relationships are the foundation (Korkusuz, 2016; Nordin & Frankel, 2012).

2.2 Implant Design in Total Knee Replacement (TKR): Basic Concepts

2.2.1 Materials in Conventional Total Knee Replacement (TKR)

In standard TKR systems, materials like cobalt-chromium-molybdenum (CoCrMo) alloys have been applied as femoral parts, titanium alloys as tibial base plates, and ultra-high molecular weight polyethylene (UHMWPE) as bearing surfaces (Korkusuz, 2016). These materials have been effective clinically for many years. On the other hand , they pose many application challenges, such as stress shielding due to modulus mismatch (Vaishya et al., 2026) and imaging artefacts (Korkusuz, 2016).

2.2.2 Total Knee Replacement: The Implant Design Landscape

In the implant design space, there has been a progress along two design trajectories, namely; monoblock and modular systems. In monoblock designs, the tibial component functions as an integrated singular product unit, made of ultra-high molecular weight polyethylene (UHMWPE), securely glued to the bone (Apostolopoulos et al., 2024). In modular designs, a metal tibial baseplate accommodates a distinct polyethylene insert, while the femoral component is usually made of cobalt-chrome alloy. The difference is clinically significant, as modularity adds extra interfaces, between the metal and the polyethylene, which create potential wear routes, absent in monoblock designs (Browne et al., 2011).

2.2.3 All-Polymer Paradigm: From Monoblock to Modular

The nomenclature around the implant designs from orthopaedic literature, clinical practice and the research domain is very challenging. But for a better understanding of the present work, this will be simplified in line with the main systems in current use.

All-polymer monoblock tibial components, have demonstrated equivalent clinical outcomes to modular metal-backed designs, at substantially lower cost (Browne et al., 2011; De Carvalho et al., 2013). This information has brought about renewed interest in all-polymer designs, for instance, in advanced healthcare systems.

Recently, progress in biomaterials, particularly PEEK OPTIMA ^{TM}, has facilitated the expansion of all-polymer designs to modular systems, that include polymer femoral components (Cowie et al., 2020; Vaishya et al., 2026). Figure 2.3 shows the distinction between the all-polymer monoblock, modular metal-backed and modular all-polymer TKR systems.

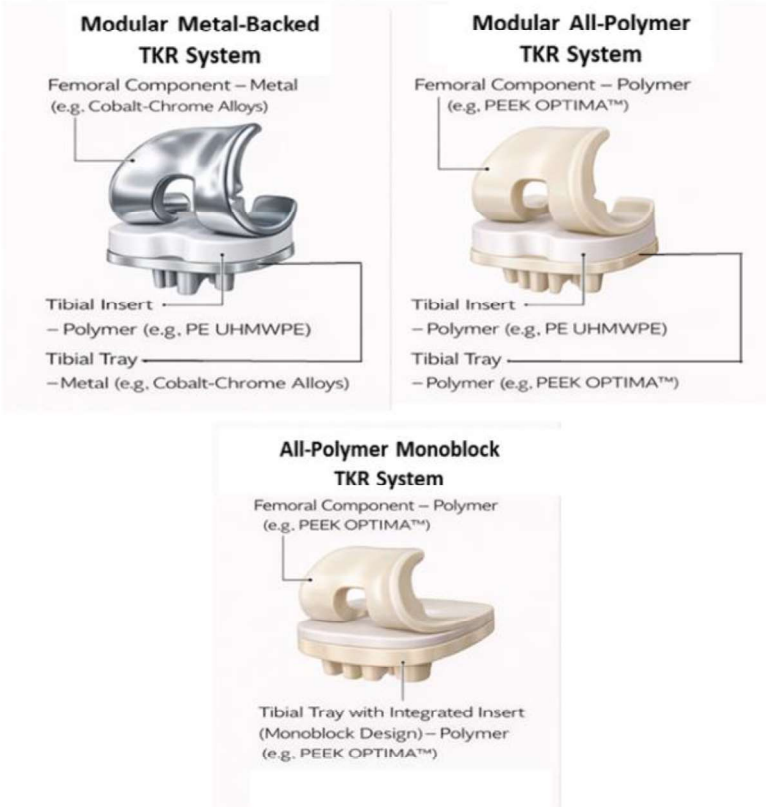


Figure 2.3. Schematic representation of different TKR design systems.
Source: Adapted from an AI-generated image produced using ChatGPT (OpenAI, 2026).

However, the modular all-polymer design, has raised new research questions about stress distribution, deformation, and wear at interfaces, not seen in monoblock systems (Browne et al., 2011; Vaishya et al., 2026). Therefore, these questions are calling for dedicated investigation.

2.2.4 An Emerging Biomaterial for Modular All-Polymer TKR Systems

Ultra-high-molecular-weight polyethylene (UHMWPE), has traditionally been the primary bearing material in TKR systems. Nonetheless, PEEK-OPTIMA™ has become a top contender for modular all-polymer TKR systems, because of its advantageous biomechanical characteristics.

The PEEK-OPTIMA™ demonstrates:

- Elastic modulus similar to cortical bone (~3–4 GPa),
- Radiolucency,
- Compatibility with biological systems,
- Resistance to chemical breakdown, (De Ruiter et al., 2017; Kurtz & Devine, 2007).

Figure 2.4 shows a human knee with implanted modular all-polymer PEEK OPTIMA ™ TKR Systems.

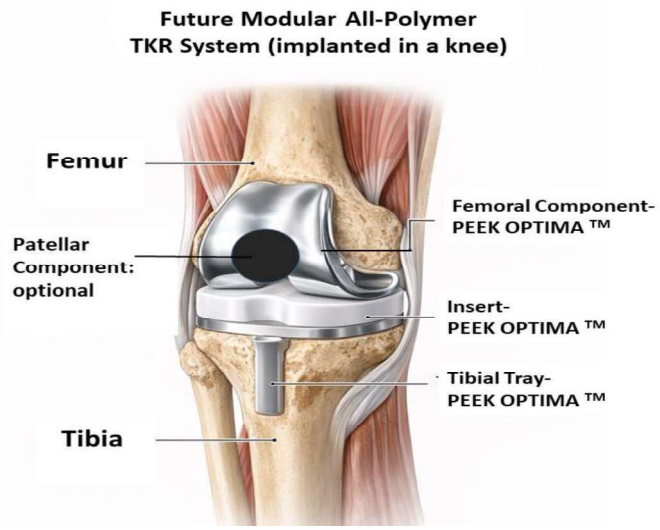


Figure 2.4. Schematic representation of Future Modular All-Polymer PEEK OPTIMA ™ TKR design systems. Source: Adapted from an AI-generated image produced using ChatGPT (OpenAI, 2026).

Recent studies have tested PEEK-OPTIMA™ polymer, in their use as tibial or femoral components, in comparison with conventional metal materials, with possible benefits, in reducing stress shielding, and compatibility with imaging (Wang et al., 2025; Zhang et al., 2023). Nevertheless, there is still concerns about PEEK-OPTIMA™ polymer wear performance under cyclic loading, especially, as long-term wear data are limited (Cowie et al., 2020, 2025).

2.3 Wear Prediction in Total Knee Replacement (TKR)

2.3.1 Mechanisms of Wear

In many total knee replacement systems, wear has been reported to occur through adhesive, abrasive, and fatigue mechanisms (Zhang et al., 2023). These mechanisms mainly affect polyethylene insert of the implant, as a result, generate debris that induce osteolysis, and aseptic loosening (Fisher et al., 2004). For the modular designs , on the other hand , the implications are significant, as they generate , backside wear at the tibial baseplate-insert interface (Wasielewski, 2002). Given that the current means of evaluating wear is expensive and costly (Abdelgaied et al., 2022), there is need to develop other means of evaluating implant longevity and performance, especially during the early design stages.

2.3.2 Archard's Wear Law: Foundation and Applications

In orthopaedic implant evaluation, the determination of wear of new joint implants are very vital since they play significant role in the longevity of prosthesis (Bartel et al., 1986). Understanding the secrets of how biological systems reduce friction, resist wear, and adapt to their environments, to deliver the expected performance , within constrained systems, are very essential for safety and efficacy compliance (A. Kumar et al., 2024).

One of the reliable tools used to model or describe wear of implants during design, is the Archard's wear law (Archard, 1953),which is an earliest model that has been used extensively, for evaluating the wear of bearing materials using finite element analysis (Delaney & Wang, 2025). Despite its simplicity, it captures the essential physical dependencies, and it has been widely used in computational wear simulations (Delaney & Wang, 2025).

In a current study by Ammarullah et al. (2026), where they examined the application of Archard's wear law, within finite element (FE) frameworks, to forecast wear in individual mobility components of total hip prosthesis under gait cycle. They observed that computational methods based on Archard's law have become valuable assets because of their versatility, affordability, and capability, to model intricate biomechanical interactions (Ammarullah et al., 2026). Although these studies showed that FE based archard´s wear models are effective, there is need to pursue data driven alternatives, since these conventional methods are limited by high computational resources , data scarcity and time (Abdelgaied et al., 2022).

Some of the developments noted by Ammarullah et al. (2026), entailed loading in multiple directions, mapping of sliding paths, and authentic material properties, to improve simulation accuracy (Ammarullah et al., 2026). Although these considerations are particularly relevant for all-polymer PEEK-OPTIMA ^{TM} TKR systems, where wear coefficients must be established for novel material combinations, this study has adopted the archard´s wear model to maintain the same effectiveness.

2.3.3 Validation Approaches in Total knee Replacement Biomechanics

To validate computer simulation studies, two main approaches have been identified from the literature namely: the ISO standard and the OrthoLoad database standard. The primary international framework , for wear testing of total knee replacements , is defined by the ISO 14243 series (Abdelgaied et al., 2022). They are based on either force (*ISO 14243-1*, 2009) or displacement (*ISO 14243-3*, 2014) control. The ISO 14243 specifies: axial force profiles, flexion–extension cycles, tibial rotation, anterior–posterior displacement, lubrication conditions, and 5 million cycle simulation benchmarks.

Many studies, however,

- Use ISO 14243-1 load-controlled protocol.
- Validate FEA wear predictions against simulator experiments.
- Report wear rates in mm^3/million cycles.

ISO loading profiles represent standardised gait cycles but may not fully reflect patient-specific or high-demand activities such as stair climbing.

The OrthoLoad database developed by Bergmann and colleagues at the Julius Wolff Institute, Charité Berlin, provides publicly available in vivo load measurements from instrumented implants (Bergmann et al., 2014) . Data include tri-axial joint contact forces, moments, and synchronized video of patient activities. This database enables researchers to validate computational models against physiological loading conditions, rather than simplified laboratory approximations (Bergmann et al., 2014).

Studies that integrate standardised testing protocols, in vivo load data, and AI-based surrogate modelling remain relatively underexplored, especially in the context of alternative polymeric tibial tray materials. The majority of existing studies focus on conventional metal-backed systems (Browne et al., 2011; De Carvalho et al., 2013). Therefore, studies of modular all-polymer PEEK-OPTIMA™ tray designs, under both ISO-defined and physiologically measured loading conditions, could make a significant contribution to the current body of knowledge.

2.4 Synthetic Data Generation in Healthcare and Engineering

2.4.1 Data Scarcity Problem in Medical Device Development

In medical device development cycle, the problem of data scarcity and restriction due to propriety rights is a big challenge. Novel implants lack historical data, making traditional machine learning approaches infeasible (Gonçalves et al., 2020). Synthetic data generation offers a pathway to create training datasets, for rare situations where data is scarce, proprietary, and private or none existent.

For this thesis, synthetic data refers to digitally generated datasets that span the design parameter space, not data learned from existing implant performance databases.

2.4.2 Statistical Methods for Parameter Exploration

The Latin Hypercube Sampling (LHS) is a sampling technique that explores multi-dimensional parameter spaces (McKay et al., 1979), efficiently. When compared to random sampling, LHS ensures that adequate coverage is achieved while minimising clusters. Laz and Browne (2010), in their comprehensive review of probabilistic methods in orthopaedic biomechanics, identified LHS as a preferred technique for implant performance analysis, due to its ability to achieve full parameter space coverage , with fewer samples than alternative methods.

2.5 Machine Learning for Regression in Biomechanics

In orthopaedic biomechanics, the application of machine learning (ML)–based regression methodologies , to characterise intricate and nonlinear associations, between mechanical loading variables and biological or material outcomes, has received new boost progressively (Chen et al., 2021; Wu et al., 2024).

Even the traditional deterministic methods, such as finite element analysis, are still fundamental, they are computationally intensive and usually inappropriate for in-depth parametric studies (Abdelgaied et al., 2022; Perrone et al., 2024).

The robustness, transparency, and reliability of these machine learning prediction models have significantly increased, due to recent advancements in statistical learning theory, and optimisation algorithms (James et al., 2013; Wu et al., 2024).

2.5.1 Random Forest

In machine learning, the Random Forest (RF), first suggested by Breiman (2001), is a type of supervised machine learning model that uses many decision trees, to make predictions. It is popular for classification or regression tasks (James et al., 2013). In biomechanical modelling, RF is particularly advantageous, because it can effectively capture nonlinear and complex interactions, without requiring prior assumptions or many data (V. Kumar et al., 2024). Also, the method can resist overfitting and noise very well and enhance interpretability in engineering applications (Han et al., 2018; Schonlau & Zou, 2020).

Recent studies have confirmed that RF models are effective in polymer implant application. In a seminal study by V. Kumar et al. (2024), they investigated the application of data driven ML models for estimating wear rate of UHMWPE inserts in hip replacement implants. Among the models compared, including Gradient Boosting, Random Forest emerged as the best-performing algorithm, achieving a mean absolute error (MAE) of 0.06, root mean square error (RMSE) of 0.17, and coefficient of determination (R^2) of 0.96, making it suitable for biomechanical estimation of polymer-based joint implants.

2.5.2 Gradient Boosting

Gradient Boosting (GB), first formalised by Friedman (2001), constitutes another highly effective family of ensemble learning techniques. In contrast to Random Forest, which builds trees independently, gradient boosting constructs models sequentially, with each successive tree trained to correct the residual errors of its predecessor. A comparative work by Grinsztajn et al. (2022), showed that gradient boosting approaches, often surpass deep neural networks on medium-scale tabula datasets, unless extensive neural network optimisation is undertaken. Contemporary implementations: including XG Boost (T. Chen & Guestrin, 2016) and Light GBM (Ke et al., 2016) have achieved state-of-the-art results on structured tabular data. While specific applications in orthopaedic wear prediction are limited, the success of these gradient boosting models are especially well known as they can manage heterogeneous feature distributions effectively (Grinsztajn et al., 2022). Accordingly, gradient boosting models represent a strong methodological candidate for predicting stress and deformation in orthopaedic implant analyses.

2.5.3 Artificial Neural Networks

Artificial Neural Networks (ANNs)(Goodfellow et al., 2016), is another kind of machine learning that is inspired from the human brain (Han et al., 2018). In biomechanics, Artificial Neural Network based multilayer perceptron (MLP) architectures have been employed for tubular data, where they have produced convincing results, such as, in works involving post-stroke patients (Lau et al., 2009) and Parkinson's disease (Wahid et al., 2015), succeeding in dealing with intricate, multidimensional data, (Horst et al., 2019).While ANNs can achieve high performance in many other tasks such as, image analysis and data augmentation (Kazeminia et al., 2019; Dindorf et al., 2024), they typically require more data and careful hyperparameter tuning than tree-based methods (Dindorf et al., 2024).

2.5.4 Comparative Model Performance

From the studies of Grinsztajn et al., (2022), the empirical evidence showed that the tree- based ML techniques frequently exceeded neural networks in both predictive accuracy and computational efficiency in moderately sized structured datasets. Nevertheless, neural architectures demonstrate superior scalability when very large synthetic datasets are available and offer greater flexibility for embedding governing physical relationships. Consequently, best practice in orthopaedic biomechanical regression involves a systematic comparative assessment of Random Forest, Gradient Boosting, and ANN models (V. Kumar et al., 2024).

2.6 Hybrid AI–Physics Modelling

One of the dangers of modelling with only data in predictive analysis, is the risk of producing results that do not obey the fundamental physical laws, governing the systems being described. In the context of medical device modelling, where patient safety is paramount, such inconsistencies are unacceptable with the regulatory bodies (Chen et al., 2021).The physics-informed machine learning methods integrate mechanistic equations with data-driven modelling to preserve physical consistency (Karniadakis et al., 2021). This integration may reduce the systems purely black-box behaviour while improving model interpretability, generalisability, and regulatory credibility.

In TKR systems, sequential hybrid approaches can, incorporate wear equations, while leveraging machine learning models to predict stress and deformation from inputs data. These

methods align with digital twin and computational screening paradigms emerging in healthcare engineering.

The present thesis adopted this sequential hybrid paradigm by:

- Using the ML models (Random Forest, Gradient Boosting, ANN), to predict contact stress and deformation, and
- Informing the Archard's wear law (physics-based) to use these predictions to compute wear volume.

This approach will ensure that the final wear predictions are grounded in established physical principles while leveraging ML's ability to capture complex parameter interactions.

2.7 Ethical and Regulatory Considerations

In medical device development, it is obligatory to ensure compliance with established ethical and regulatory frameworks. The General Data Protection Regulation (GDPR) governs the handling of personal data within the European Union (European Parliament & Council, 2016, Art.5). Although the present study used fully synthetic data, reproducibility and transparency remained important throughout the study.

In the study, the transparent documentation of synthetic data generation and model parameters was implemented through excel format, data and model cards, to enhance reproducibility, in line with the FAIR principles , which require that research data should be Findable, Accessible, Interoperable, and Reusable (Wilkinson et al., 2016). The European Union Artificial Intelligence Act (European Parliament & Council, 2024, Art. 9 -10), has designated medical AI systems as high-risk technologies, thereby requiring comprehensive risk management procedures, high-quality datasets, technical documentation, transparency measures, and meaningful human oversight. While early-stage research frameworks, are not directly classified as high-risk medical devices, alignment with transparency and documentation standards supports responsible AI development.

2.8 Research Gaps and Positioning of This Work

Existing literature demonstrates:

- Extensive reliance on experimental and FEA-based implant validation.

- Growing application of machine learning in biomechanics.
- Limited integration of synthetic data generation with physics-informed wear modelling for modular all-polymer PEEK- OPTIMA ^{TM} knee trays.

Few studies combine:

- Multidimensional synthetic sampling,
- Machine learning regression for stress/deformation prediction,
- Archard-based wear modelling,
- Dual validation against ISO standards and in vivo OrthoLoad envelopes.

This study addresses this gap, by developing a unified digital framework capable of early-stage screening of PEEK- OPTIMA ^{TM} based tibial components, using synthetic data and hybrid modelling.

2.9 Theoretical and Analytical Framework

The theoretical and analytical structure of this work are given below:

1. Classical contact mechanics (Bartel et al., 1986; Nordin & Frankel, 2012),
2. Tribological wear theory (Archard, 1953),
3. Statistical learning principles (James et al., 2013).

The theoretical foundation for stress estimation is based on basic connection between applied load, contact area, and material stiffness(Nordin & Frankel, 2012). Deformation is modelled using the basic interactions between elastic strain , stress and material modulus mathematically (Nordin & Frankel, 2012).

The wear calculation is based on Archard's wear law, which relates wear volume to applied load, sliding distance, wear coefficient, and material hardness (Archard, 1953). This formulation provides, the physical basis for the cumulative wear modelling, within the digital framework.

The analytical implementation combines these physics-informed formulations with supervised machine learning regression models, such as Random Forest, Gradient Boosting, and Artificial Neural Networks. These models are grounded in statistical learning theory and are designed to deal with nonlinear mappings between input parameters and biomechanical

outputs (James et al., 2013). Figure 2.5 demonstrates the theoretical and analytical frame work of the study.

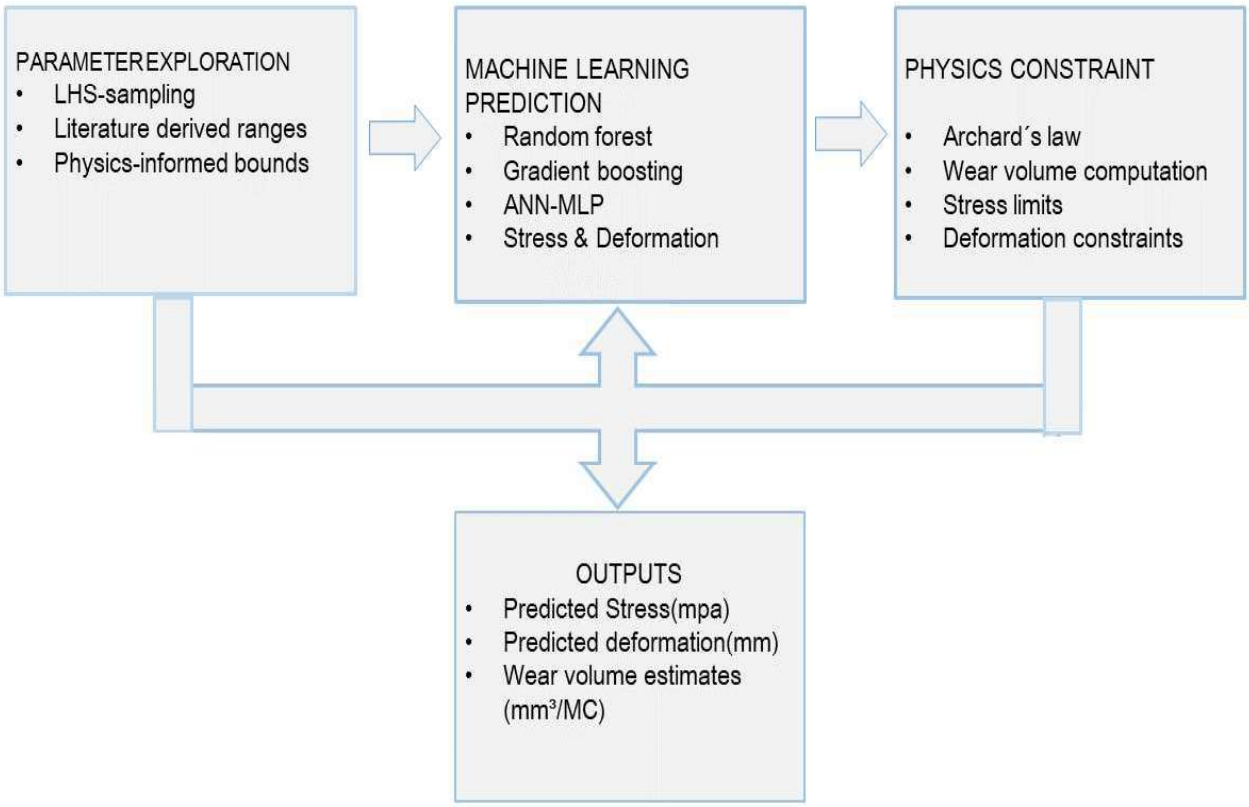


Figure 2.5 The theoretical and analytical framework of the study. Source: Author´s own work (2026).

Together, this hybrid framework integrates deterministic physical relationships with data-driven predictive modelling to enable digital simulation of implant biomechanics.

Chapter 3
Methodology

3.1 Overall Workflow

This study adopted a quantitative, physics-informed, data-driven methodology for predicting biomechanical stress, deformation, and wear in modular all-polymer knee trays manufactured from PEEK-OPTIMA™.

The methodological approach combined synthetic data generation, machine learning surrogate modelling, and physics-based wear estimation into a single reproducible digital pipeline.

In addition, the methodology did not include finite element analysis (FEA) and physical experimentation intentionally, but rather it concentrated on exploratory, surrogate, decision-support objective of early-stage digital screening of implant designs.

The overall workflow was executed in seven (7) major steps:

(1) Definition of biomechanically relevant geometry, material and loading parameter ranges.

(2) Synthetic datasets generation using Latin Hypercube Sampling (LHS).

(3) Computation of stress and deformation outputs using simplified physics-informed relationships.

(4) Exploratory Data Analysis (EDA) for statistical and biomechanical plausibility.

(5) Supervised machine learning models training for biomechanical behaviour prediction.

(6) Hybrid wear estimation using Archard's wear equation.

(7) Validation against standardised and in vivo loading benchmarks as well as documentation under FAIR and GDPR framework to ensure ethical compliance and reproducibility, as shown in Figure 3.1.

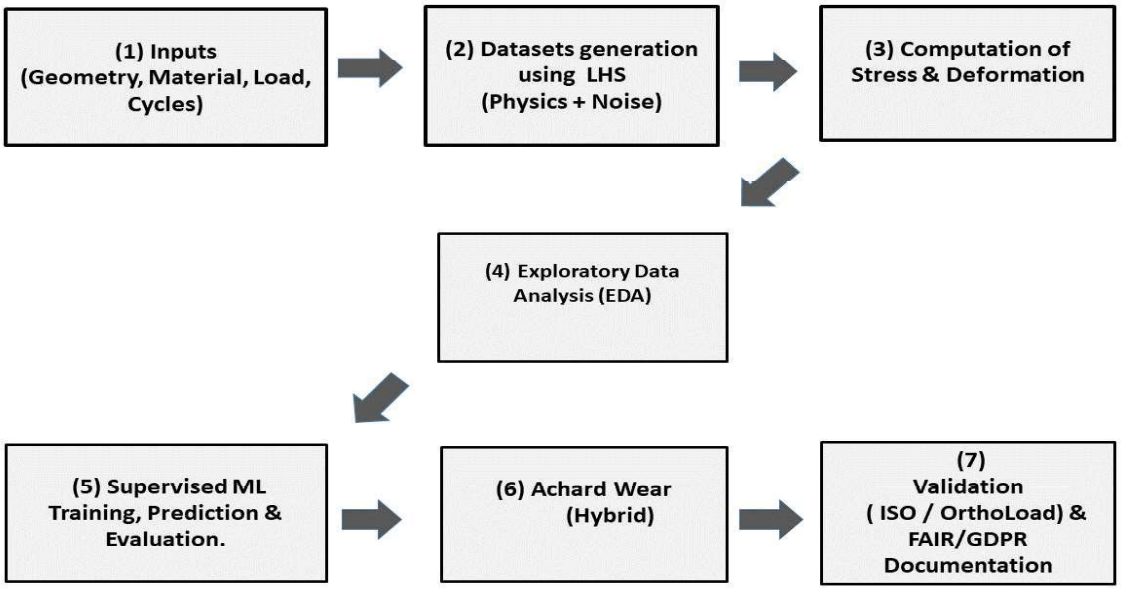


Figure 3.1 Digital Pipeline Overview. Source: Author´s own work (2026).

This workflow ensures that data-driven predictions remain grounded in well-known established physical principles while ensuring early-stage screening of implant designs without requiring finite element analysis or experimental wear testing , maintaining computational efficiency and reproducibility (Chen et al., 2021).

3.2 Synthetic Data Generation

3.2.1 Parameter Definition

Before the synthetic data generation, the parametric design space, that is representative of all-polymer knee trays, was defined numerically based on biomechanical importance, and availability in the literature. Input parameters were defined based on reported biomechanical ranges for total knee replacements and material properties of PEEK-OPTIMA ^{TM} (Kurtz & Devine, 2007) . The following parameters were included: thickness (mm), contact area (mm²), elastic modulus (GPa), poisson's ratio, axial load (N), friction coefficient, sliding distance per cycle (mm), hardness (MPa), wear coefficient , and number of loading cycles.

The loading magnitudes were chosen, to align with physiological knee forces reported in the OrthoLoad database(Bergmann et al., 2014), and within the envelope of ISO 14243 knee wear testing standards (*ISO 14243-1*, 2009; *ISO 14243-3*, 2014).The ranges were intentionally made broad to support screening-level exploration rather than exact device replication, as shown in table 3.1.

Table 3.1. Input Parameter Ranges Used in the Synthetic Data Generation

Parameter	Range Used	Unit	Rationale	Source
Inputs				
Tibial tray thickness	6 – 14	mm	Typical polymer insert thickness in TKR systems	(Kindel et al., 2025; Massin, 2017)
Curvature radius	20 – 60	mm	Typical femoral condyle radii range in knee prostheses	(Chaurasia et al., 2021)
Contact area	600 – 1200	mm^2	Typical tibial contact areas under load	(Triwardono et al., 2021)
Elastic's modulus (PEEK)	3 – 5	GPa	Reported modulus of PEEK-OPTIMA	Kurtz & Devine (2007)
Poisson's ratio (PEEK)	0.35 – 0.42	–	Published values for medical-grade PEEK	(De Ruiter et al., 2017)
Hardness	150 – 300	MPa	Typical hardness range for PEEK materials	(*PB30900 Data Sheet | Industrial Plastic Solutions | PBY Plastics*, n.d.; Shive, n.d.)
Axial load	500 – 3000	N	Walking loads up to 3× body weight	(Bergmann et al., 2014; *ISO 14243-3*, 2014)
Sliding distance per cycle	0.5 – 5	mm	Typical knee joint sliding distances	(*ISO 14243-3*, 2014)
Cycles	$1\times10^5 – 5\times10^6$	–	Standard knee wear test cycles	(*ISO 14243-3*, 2014)
Outputs	Stress (Mpa)		Deformation (mm)	Wear (mm^3/MC)

However, Since the parameters were specified numerically, instead of geometrically, the approach bypasses mesh-based models, while effectively reflecting significant biomechanical diversity (Chen et al., 2021).

3.2.2 Latin Hypercube Sampling

The Latin Hypercube Sampling (LHS), was employed to generate 8000 synthetic biomechanical datasets, in order to utilise and explore the multi-dimensional parameter space efficiently.

The Latin Hypercube Sampling (LHS), is a stratified sampling technique, that is applied to ensure that, the coverage of each parameter range is uniform, while ensuring minimal utilisation of the total number of samples required (McKay et al., 1979).

This means that each synthetic sample aligns, to a particular combination of implant parameters and loading conditions, forming the basis or ground truth, for subsequent biomechanical proxy calculations (Behnam et al., 2024; Kleist et al., 2025).

The final synthetic biomechanical datasets were made of 8000 rows and 13 variables.

3.2.3 Physics-Informed Stress and Deformation Estimation

Since no finite element simulations were carried out, biomechanical outputs such as stress and deformation were generated using physics-informed proxy equations rather than numerical solvers. The stress was computed using a simplified contact mechanics proxy equation given below as:

$$\sigma \propto \frac{F}{A} \qquad \text{.....3.1}$$

Where **F** represents axial load and **A** represents contact area (Bartel et al., 1986).

For the deformation, it was estimated based on elastic strain theory:

$$\epsilon \propto \frac{\sigma}{E} \qquad \text{.....3.2}$$

Where E is elastic modulus. These formulations preserve first-order mechanical dependencies between load, contact area, stiffness, and deformation (Nordin & Frankel, 2012).

Although these equations were simplified relative to finite element modelling, these relationships maintain physical plausibility within the defined screening scope.

Controlled stochastic noise of 5% and 8% were added to the stress and deformation proxy outputs respectively , to enhance realism and hinder over-deterministic behaviour(Zhu et al., 2025). This approach agrees with best practices in synthetic data generation, where variability is introduced to better approximate real-world uncertainty while preserving physical plausibility (Zhu et al., 2025). In implant research, It accounts for the experimental noises and variability observed with wear studies (Cowie et al., 2025).

3.2.4 Exploratory Data Analysis

Before the model training, exploratory data analysis was carried out to examine the following:

i) Dataset completeness (absence of missing or invalid values),
ii) Range compliance,
iii) Pairwise correlations,
iv) Distribution smoothness,
v) Monotonic trend consistency.
vi) Presence of statistical outliers using the interquartile range (IQR) method.

Also, to confirm the expected physical trends, spearman rank correlation coefficients were implemented to asses monotonic associations between the variables, given the nonlinear nature of some interactions, (James et al., 2013).

These checks are vital to ensure that the synthetic datasets are consistent with biomechanical expectations in terms of quality and other factors, despite being fully artificial, reflecting the exploratory and screening-oriented nature of the framework.

3.3 Machine Learning Models for Biomechanical Prediction

3.3.1 Feature Selection

The features that were chosen for the study were geometric parameters, material properties, and loading conditions. Based on their direct influence on stress and deformation behavior, these features were chosen, to agree with the classical mechanics principles (Bartel et al., 1986; Nordin & Frankel, 2012).

The target variables were:

- Stress (MPa).
- Deformation (mm).
- Wear (mm^3/MC).

3.3.2 Model Selection

Three supervised machine learning models were implemented and compared in the study. They are namely:

1. Random Forest (RF): – ensemble of decision trees using bootstrap aggregation (Breiman, 2001). Chosen for Its robustness to nonlinear relationships and noise (Han et al., 2018; Schonlau & Zou, 2020).
2. Gradient Boosting (GB): – sequential tree-based boosting model (Friedman, 2001). Chosen for its strong predictive performance on structured tabular data (Grinsztajn et al., 2022).
3. Artificial Neural Networks (ANNs):-feedforward artificial neural network (Goodfellow et al., 2016). Implemented as multilayer perceptrons to model intricate interactions between parameters (Han et al., 2018).

3.3.3 Training and Hyperparameter Tuning

Models were trained using an 80/20 train–test split. The hyperparameter tuning was performed using randomised search with cross-validation. The performance was evaluated and compared using: the Root Mean Squared Error (RMSE), the Mean Absolute Error (MAE), and the Coefficient of Determination (R^2). For regression model evaluation (James et al., 2013), these metrics are normally used to quantify predictive accuracy and variance explanation.

3.4 Hybrid Wear Prediction Model

The wear estimation was performed using Archard's wear equation, a widely adopted model for estimating material loss in sliding contacts (Archard, 1953):

$$V = k (F \cdot S) / H \quad \text{.....3.3}$$

Where: **V** is the wear volume, **K** is the wear coefficient, **F** is the applied load, **S** is the total sliding distance, **H** is material hardness and **S** is sliding distance per cycle was multiplied by total cycles to compute cumulative wear. Despite its simplification, and inability to account for all tribological processes, Archard's law is appropriate for trend analysis and relative wear estimates in orthopaedic applications (Delaney & Wang, 2025).

3.4.1 Sensitivity Analysis

One-at-a-time (OAT) parametric sweeps were conducted to evaluate wear sensitivity to axial load. In each sweep, a single parameter was varied while others were held constant. This approach isolates parameter influence and supports causal interpretation.

3.5 Validation Approach

Validation was conducted at a trend and consistency level, rather than through direct numerical comparison with experimental results.

3.5.1 ISO 14243 Benchmarking

The synthetic loading magnitudes were compared against ISO 14243 gait cycle envelopes, which defined standardised loading conditions for knee wear testing(*ISO 14243-1*, 2009; *ISO 14243-3*, 2014).The synthetic load range was selected to overlap with this envelope.

3.5.2 OrthoLoad Dataset Comparison

In order to ensure biomechanical plausibility, load magnitudes were also contrasted with in vivo knee joint forces documented by Bergmann et al. (2014), using instrumented implants, which are publicly accessible OrthoLoad datasets (Bergmann et al., 2014).

3.5.3 Performance Evaluation

The model accuracy was assessed using RMSE, MAE, and R^2. This evaluation approach is not numerically equivalent to experimental stress measurements. It only shows trend-level

consistency and envelope alignment (Nordin & Frankel, 2012). This strategy ensures that the known biomechanical parameters are intact while being consistent with the digital-only scope of the study (Nordin & Frankel, 2012).

3.6 Ethical and Reproducibility Measures

To ensure that the study is compliant with the General Data Protection Regulation (GDPR) and to eliminate patient privacy concerns, all the datasets generated in this study were entirely synthetic. No confidential, personal, or patient-derived data was used. Synthetic biomechanical datasets avoid the privacy, regulatory, and proprietary concerns commonly associated with orthopaedic testing data (Chen et al., 2021). To make the work reproducible, it was supported through the following: open-source python implementation, version-controlled scripts, documentation using data cards and model cards and transparent parameter reporting.

During the organisation of the datasets and code, the FAIR principles guideline was adopted: that is to make the data and code , findable, accessible, interoperable, and reusable by anyone who intends to obtain the same results (Wilkinson et al., 2016). The development of Data Cards and Model Cards, which record the origin of datasets, model assumptions, intended use, and restrictions, further improves transparency of the study (Mitchell et al., 2019).

3.7 Tools and Implementation Environment

The full methodology was implemented in Python 3.11 using open-source scientific libraries:

- NumPy and Pandas for data manipulation
- Scikit-learn for machine learning models
- Matplotlib for visualization
- Joblib for model serialisation

The study was conducted in Jupyter Notebooks within a Google Colab environment. This is because of reproducibility and ease of access. Version control is managed using Git, and all code, documentation, and results are structured to support open scientific practice. All outputs, including datasets, trained models, and figures, were exported for documentation.

Chapter 4
Results

4.1 Synthetic Dataset Characteristics and Exploratory Analysis

4.1.1 Dataset Overview

In data science, EDA is always done to ensure that high quality data are obtained, before the modelling process (James et al., 2013). The synthetic dataset of 8000 samples and 13 variables, was generated using Latin Hypercube Sampling, to ensure good coverage of the predefined parameter ranges.

The final dataset, contained several thousand samples, each representing a unique combination of implant geometry, material properties, and loading conditions. All input parameters remained within the defined design space boundaries as given in table 4.1.

Table 4.1. Descriptive Statistics of Synthetic Dataset Variables

Variables	Count	Mean	Std	Min	25%	50%	75%	Max
Thickness (mm)	8000	10	2.309541	6.00019	8.000037	10.00015	11.99959	13.99967
Curvature_radius (mm)	8000	39.99998	11.54775	20.00254	30.00017	40.00092	49.99823	59.99748
contact_area (mm^2)	8000	900	173.2155	600.07	750.0067	900.0047	1050	1199.967
Elastic Modulus (Gpa)	8000	4.000001	0.577386	3.000147	3.500009	3.999997	4.499941	4.999901
Poisson's ratio	8000	0.385	0.020208	0.350006	0.367503	0.385	0.402495	0.419995
Hardness (Mpa)	8000	225	43.30394	150.0054	187.5121	225.0034	262.4983	299.9813
Axial_load (N)	8000	1749.998	721.7348	500.0726	1125.148	1750.067	2374.845	2999.706
Sliding (mm /cycle)	8000	2.749999	1.299117	0.500372	1.625013	2.750158	3.87504	4.999619
Cycles	8000	1235760	1269747	100123	261083	691268.5	1851915	4999550
Stiffness_proxy	8000	0.423386	0.121426	0.216626	0.331002	0.399716	0.497851	0.825087
Stress (Mpa)	8000	2.059153	0.994912	0.388639	1.260384	1.951812	2.720854	5.776519
Deformation (mm)	8000	0.027873	0.016261	0.003475	0.015686	0.024468	0.036468	0.110369
Wear (mm^3/million cycles)	8000	2.72867	3.91046	0.021605	0.435589	1.179382	3.293262	45.06675

The descriptive statistics showed that the distributions of thickness, contact area, load, elastic modulus, hardness, and sliding distance were approximately uniform, as expected from the sampling method, as given in figure 4.1.

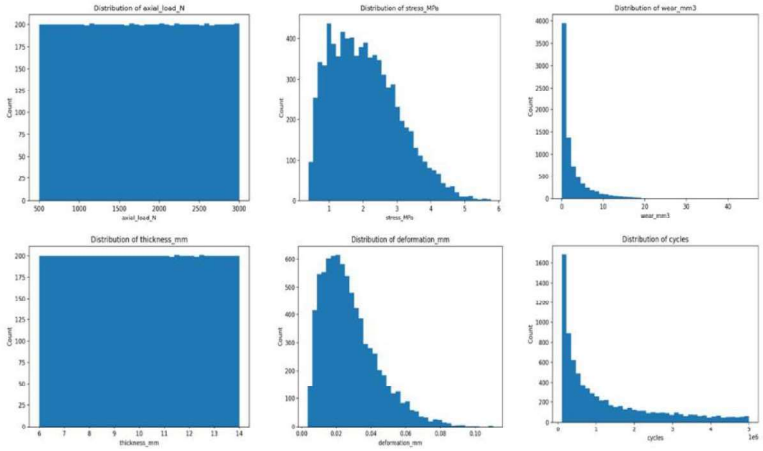


Figure 4.1. Distribution of key input and output variables in the synthetic dataset. Source: Author´s own work (2026).

This confirms that the design space was properly explored in a balanced way without any clustering regions.

4.1.2 Correlation Analysis

To evaluate the monotonic relationships among variables, the spearman rank correlation analysis was carried out. The correlation analysis showed a strong positive association between the axial load and stress (r = 0.859), as well as between the stress and deformation (r = 0.819). The deformation also revealed a strong correlation with axial load (r = 0.709). These trends align with expected mechanical behaviour in load-bearing systems (Nordin & Frankel, 2012), as shown in figure 4.2.

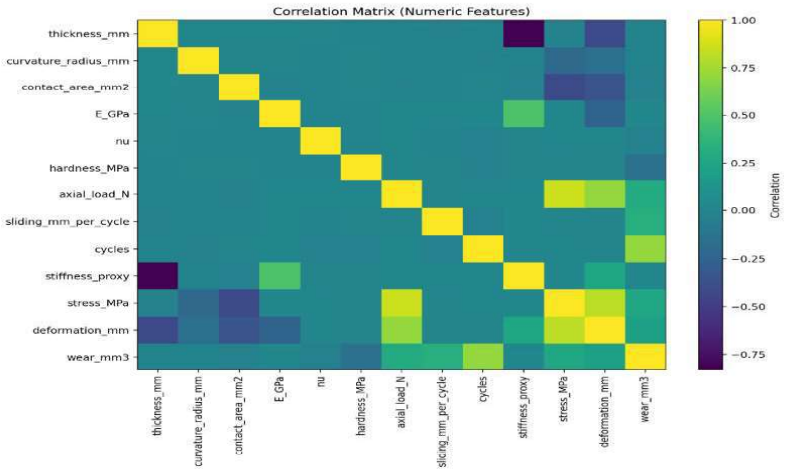


Figure 4.2. Spearman rank correlation matrix of input parameters and predicted biomechanical outputs in the synthetic dataset. Source: Author´s own work (2026).

Figure 4.2 shows a significant positive correlation (r = 0.708) between the loading cycles and the wear findings, indicating cumulative wear behaviour (Li & Ma, 2022). There was a moderate correlation between the contact area and stress (r = 0.419). This is consistent with the consequences of multidimensional sampling. The majority of cases caused mild wear, but fewer extreme loading combinations created greater wear values, according to the wear distribution's right skewness (skewness = 3.008).

For the interquartile range (IQR) analysis, 41 potential outliers for stress, 203 for deformation, and 776 for wear, were discovered respectively. The higher outlier count for wear reflects its multiplicative, cumulative formulation and noise associated with biological systems (Li & Ma, 2022).

Since this study was completely digital, and does not include real patient data, a direct real-versus-synthetic comparison was not possible. However, the relevant parameter ranges were chosen based on literature values reported for knee joint loading, PEEK polymer properties, and wear testing standards (Bergmann et al., 2014; Kurtz & Devine, 2007; (*ISO 14243-1*, 2009; *ISO 14243-3*, 2014).

In general, the exploratory data analysis confirmed, the statistical stability, and biomechanical relevance of the generated dataset. The synthetic datasets showed sufficient variability, physical consistency, and numerical robustness to support reliable machine learning model training.

4.2 Model Performance for Stress and Deformation Prediction

Three supervised regression models were implemented and evaluated for predicting stress and deformation namely:

- Random Forest (RF)
- Gradient Boosting (GB)
- Artificial Neural Network (ANN)

The models were trained using an 80/20 train-test split. Performance was evaluated using root mean squared error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2).

4.2.1 Stress Prediction

The objective of the stress prediction task, was to develop a machine learning surrogate model, capable of estimating contact stress based on geometric, material, and loading parameters.

The stress values, used as training targets, were generated, using physics-informed proxy equations. Though they were derived from load-to-contact-area relationships, they were consistent with the classical contact mechanics principles (Bartel et al., 1986).The stress prediction performance of the three models is given in table 4.2.

Table 4.2. Performance Metrics for Stress Prediction Models

Target	Model	RMSE	MAE	R^2
Stress (MPa)	Random Forest	0.130	0.094	0.983
	Gradient Boosting	**0.126**	**0.093**	**0.984**
	ANN	0.138	0.104	0.981

The results of the model evaluation, showed that all the three models achieved high predictive accuracy for stress estimation. Gradient Boosting achieved the lowest RMSE (0.126 MPa), and the highest R^2 (0.984), indicating very strong predictive performance. Random Forest trailed closely behind with similar accuracy (R^2 = 0.983), and the ANN also performed well (R^2 = 0.981), suggesting that the three model types successfully learnt and captured stress correlations. Figure 4.3 presents the predicted versus proxy stress values for the best-performing model.

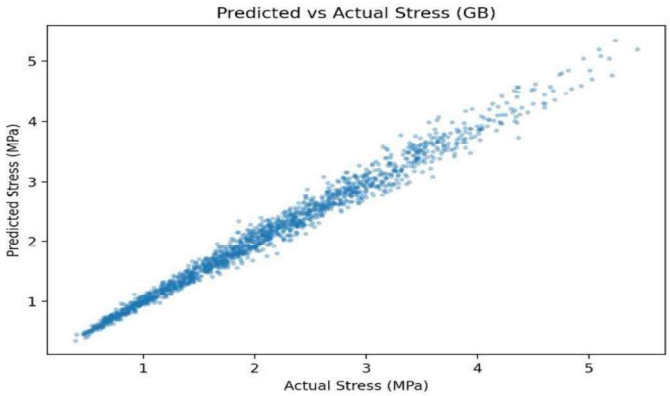


Figure 4.3. Predicted versus proxy (Actual) stress values for the selected surrogate model. Source: Author´s own work (2026).

The predicted-versus-actual scatter plots showed tight clustering around the identity centre, indicating good agreement between proxy labels and predictions.

Feature importance analysis (from the Random Forest model), was performed to identify the most significant parameters for stress prediction. The results indicated that load, contact area, and thickness were the most influential parameters for stress prediction as shown in figure 4.4.

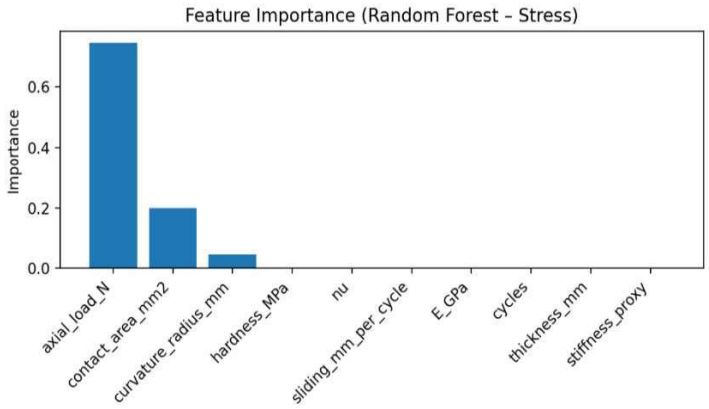


Figure 4.4. Relative feature importance for stress prediction derived from the Random Forest model. Source: Author´s own work (2026).

This ranking supports the interpretability of the surrogate model (Payne et al., 2013) and is biomechanically justifiable , as stress in contact systems is mainly controlled by applied force and contact area (Bartel et al., 1986).

Overall, the stress prediction models, showed a strong accuracy and stable generalisation performance. Within a synthetic data environment (Ammarullah et al., 2026), machine learning models, may efficiently learn nonlinear relationships, that are present, between implant parameters and stress proxies, as confirmed by the findings.

According to Payne et al. (2013), these results provide credence, to the use of surrogate modelling as an early screening method before high-fidelity simulation or experimental testing.

4.2.2 Deformation Prediction

For the second prediction task, the deformation of the knee tray under applied loading conditions, was estimated. The deformation values, were obtained from a physics-informed proxy model, based on simplified elastic strain relationships, where deformation was proportional to stress and inversely related to elastic modulus. Thickness and geometric compliance effects, were also incorporated. This approach, reflects basic elastic theory

principles, where strain is proportional to stress divided by material stiffness (Nordin & Frankel, 2012). For the deformation prediction, similar trends were observed as shown in table 4.3.

Table 4.3. Performance Metrics for Deformation Prediction Models

Target	Model	RMSE	MAE	R^2
Deformation (mm)	Random Forest	0.00386	0.00263	0.946
	Gradient Boosting	0.00359	0.00241	0.954
	ANN	0.01625	0.01264	0.048

From the deformation prediction metrics of the models , a resilient performance was shown, by the Gradient Boosting , due to negligible prediction error and uniform generalisation (R^2 = 0.954), which was closely replicated by Random Forest (R^2 = 0.946). On the other hand, the ANN exhibited significantly inferior prediction performance (R^2 = 0.048), signifying restricted generalisation capacity for this target.

4.3 Wear Estimation Results

Wear was estimated using Archard's wear law, which relates wear volume to load, sliding distance, material hardness, and wear coefficient (Archard, 1953). Table 4.4 shows the wear prediction performance of the model.

Table 4.4. Performance Metrics for Wear Prediction Model

Metric	Value	**Interpretation**
RMSE (mm^3/MC)	2.47	On average, the predicted wear deviates by ~1 mm^3 from the reference value
MAE (mm^3/MC)	1.03	Larger errors occur occasionally due to cumulative and non-linear wear behaviour
R^2	0.586	The model explains ~59% of the variability in wear trends

The wear prediction model achieved an RMSE of 2.47 mm^3 per million cycles and an MAE of 1.03 mm^3 per million cycles, with an R^2 value of 0.586. These results indicate moderate predictive performance compared to stress and deformation models.

The hybrid wear model, where the wear coefficient was mildly influenced by predicted stress, showed slightly greater sensitivity in high-stress conditions as shown in figure 4.5.

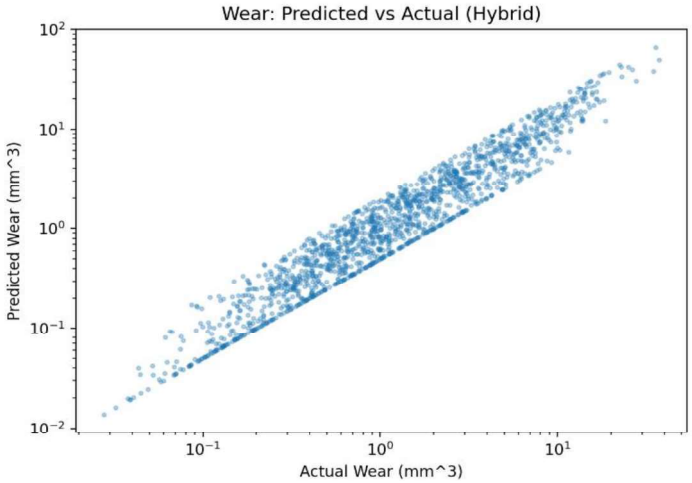


Figure 4.5. Hybrid wear model, where the wear coefficient was mildly influenced for stress prediction derived from the Gradient Boosting model. Source: Author´s own work (2026).

However, the overall behavior remained stable and physically consistent. On the other hand the, the result of one-time-sweep for axial load against wear showed an increasingly rise, confirming the systems responsiveness.

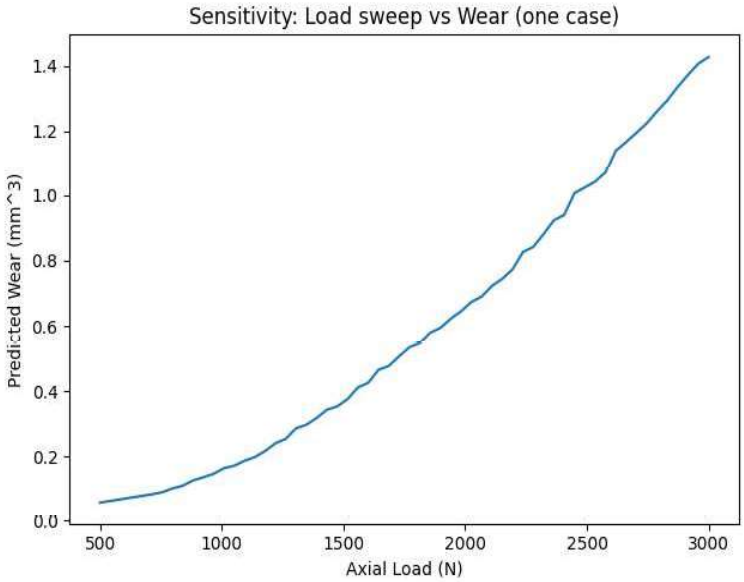


Figure 4.6. Sentivity sweep of axial load against wear. Source: Author´s own work (2026).

4.4 Validation of the Digital Framework

To validate the digital framework, a structured multi-layered approach was designed to assess physical consistency, behavioural stability, external generalisation, and robustness across implant design variability. Rather than relying solely on statistical performance metrics, validation was structured to focus on consistency with published loading standards, and alignment with reported biomechanical magnitudes, to ensure biomechanical interpretability and engineering reliability of the digital workflow. Since the dataset is fully synthetic and no experimental calibration was performed, validation emphasised envelope comparison and trend verification rather than direct experimental accuracy.

4.4.1 Validation Layer 1: Physical Consistency and Parametric Sensitivity Validation

Prior to external validation, the digital framework was evaluated for physical consistency through parametric sensitivity analysis. The objective of this step was to ensure that model predictions align with established biomechanical principles, rather than merely reflecting statistical fitting performance (Delaney & Wang, 2025). Axial load, implant thickness, and cycle count were independently varied , while holding the other remaining parameters constant, to assess monotonic and physically interpretable behaviour (Nordin & Frankel, 2012). Predicted stress increased monotonically with axial load, as shown in figure 4.7.

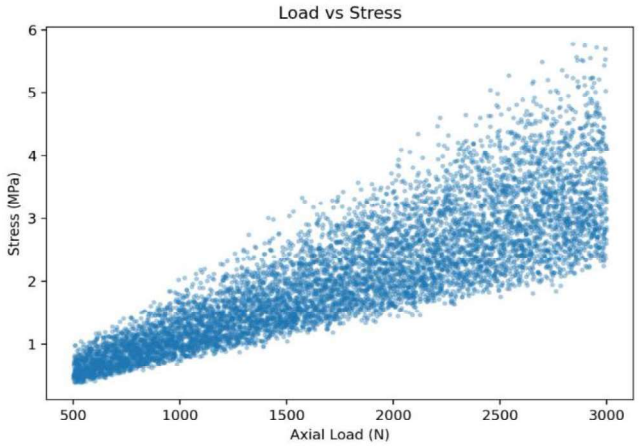


Figure 4.7. Stress vs Axial Load (monotonic curve). Source: Author´s own work (2026).

This agrees with the classical contact mechanics, where contact stress is proportional to applied normal force (Bartel et al., 1986). Similarly, the predicted deformation decreased , as implant thickness increased, reflecting increased structural stiffness, and reduced compliance under loading, as given in figure 4.8.

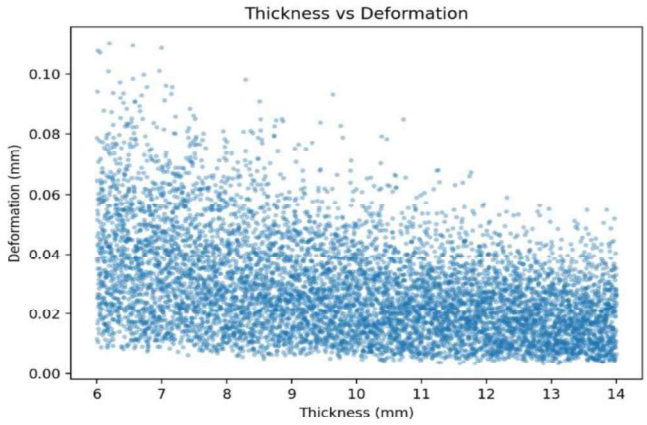


Figure 4.8. Deformation vs Thickness. Source: Author´s own work (2026).

This trend aligns with fundamental mechanical theory, governing elastic deformation in load-bearing components (Nordin & Frankel, 2012).

In addition, wear predictions demonstrated, proportional growth with increasing cycle count figure 4.9.

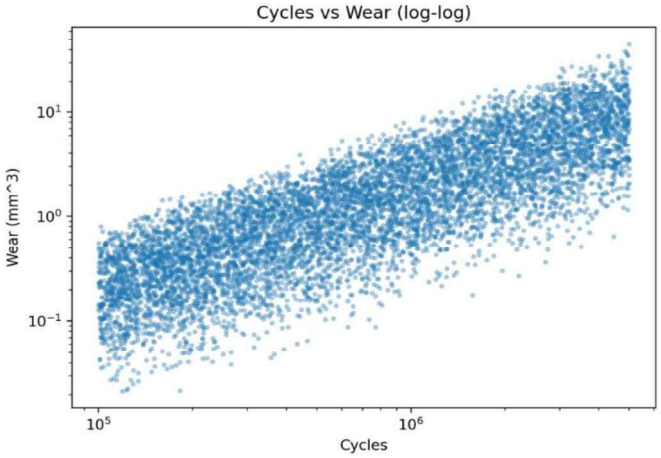


Figure 4.9. Wear vs Cycles. Source: Author´s own work (2026).

This agrees with Archard's wear law, which defines wear volume as directly proportional to normal load and sliding distance over repeated cycles (Archard, 1953).

These sensitivity results, confirm that the model preserves essential mechanical relationships governing stress, deformation, and wear in modular all-polymer-based knee implants (Nordin & Frankel, 2012). Establishing physical consistency, prior to behavioural and external validation , strengthens confidence in the interpretability and engineering reliability of the digital workflow (Payne et al., 2013).

4.4.2 Validation Layer 2: ISO-like Gait Load Behavioural Validation

Following confirmation of physical consistency through parametric sensitivity analysis, behavioural validation was performed using an ISO-informed gait loading profile. The axial load waveform was constructed to reproduce the characteristic double-peak pattern observed during physiological walking and described in knee wear testing standards (*ISO 14243-1*, 2009; *ISO 14243-3*, 2014). Although simplified, the waveform reflects the magnitude range and temporal structure, typically applied in simulator-based wear evaluations (Abdelgaied et al., 2022).

To evaluate behavioural consistency, under physiologically structured loading, an ISO-like gait force profile was applied to a representative implant configuration while geometric and material parameters were held constant. The loading curve was defined over a normalized gait cycle (0–100%) and constructed to replicate the characteristic double-peak axial load observed in knee joint biomechanics as shown in figure 4.10.

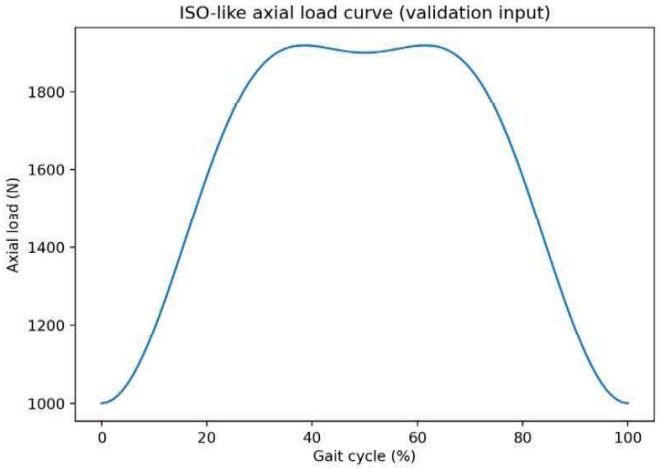


Figure 4.10. ISO-like gait curve validation for a representative implant configuration. Source: Author´s own work (2026).

The trained Gradient Boosting model was used to predict stress at each time step of the gait cycle figure 4.11, while wear was estimated using the hybrid AI–physics framework based on Archard's law figure 4.12.

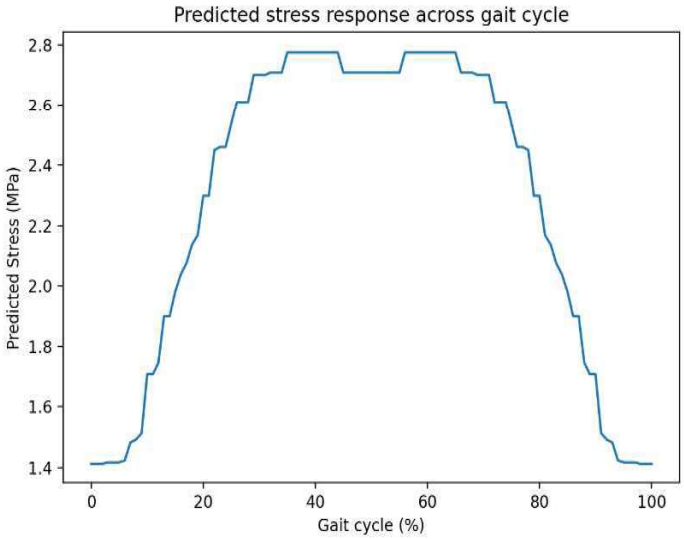


Figure 4.11. Predicted stress response for a representative implant configuration across gait cycle. Source: Author´s own work (2026).

The predicted stress response exhibited clear alignment with the applied loading peaks, demonstrating a monotonic and physically consistent load–response relationship.

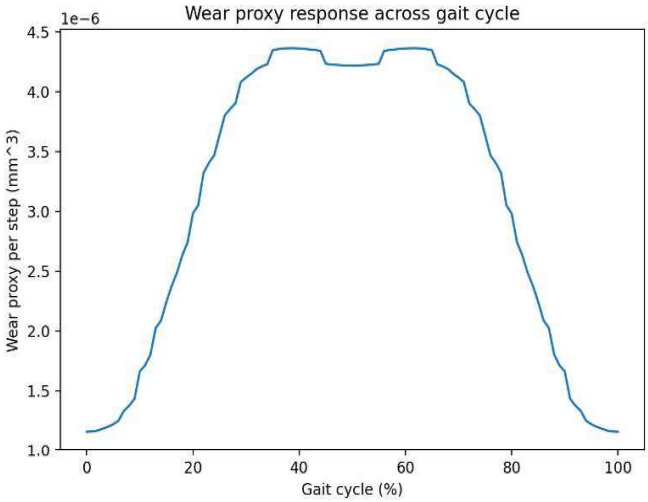


Figure 4.12. Predicted wear proxy response for a representative implant configuration across gait cycle. Source: Author´s own work (2026).

The corresponding wear proxy showed, high values during peak loading phases, consistent with the proportional dependence defined by Archard's wear law (Archard, 1953). These findings indicate that the learned model preserves expected biomechanical behaviour when exposed to structured, non-random loading patterns, beyond the training distribution.

Figure 4.13 presents an overlay comparison, between the ISO-like axial load waveform, and the in-vivo OrthoLoad resultant force profile.

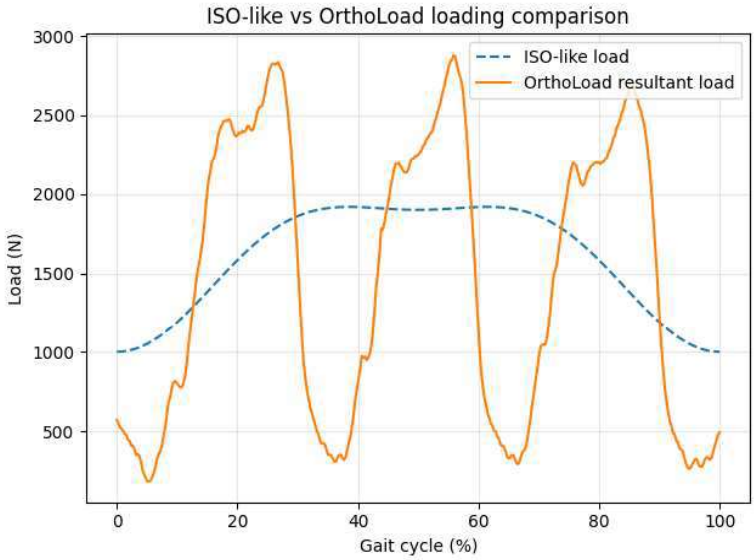


Figure 4.13. Comparison of ISO-like and OrthoLoad gait loading profiles. Overlay of the synthetic ISO-like axial load waveform and the in-vivo resultant force magnitude obtained from the OrthoLoad database (Bergmann et al., 2014), both normalised over the gait cycle. Both curves exhibit the characteristic double-peak structure associated with physiological walking, supporting the use of the ISO-like waveform for behavioural validation and OrthoLoad as external validation. Source: Author´s own work (2026).

Both curves exhibit, the characteristic double-peak pattern, associated with physiological walking. While the absolute magnitudes differ slightly, the temporal structure is preserved. This comparison supports, the suitability of the ISO-like waveform, as a simplified behavioural validation input, and establishes continuity, between conceptual and external validation stages.

4.4.3 Validation Layer 3: External Validation Using OrthoLoad

To assess generalisation, beyond synthetic training conditions, in-vivo knee joint force data, from the OrthoLoad database (Bergmann et al., 2014), were applied to the trained model without retraining or recalibration. The OrthoLoad dataset, provides experimentally measured joint forces recorded, from instrumented knee implants, during physiological walking (Bergmann et al., 2014). Figure 4.14 presents, the resultant force magnitude computed from the measured three-dimensional force components, which was normalised over the gait cycle. This loading profile, was used as a time-varying input, while all geometric and material parameters were held constant for a representative implant configuration.

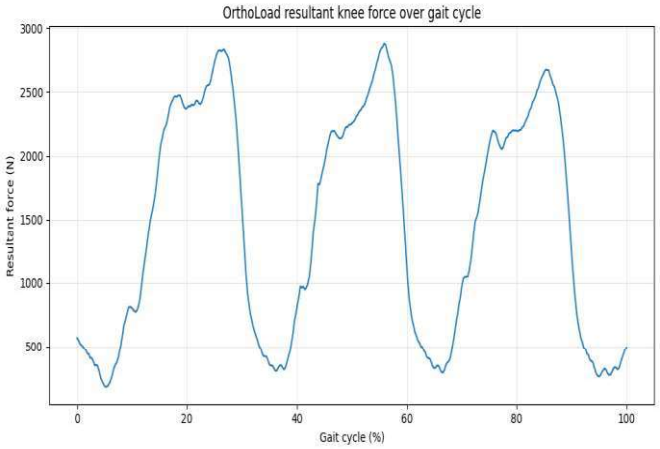


Figure 4.14. OrthoLoad in-vivo knee joint resultant force over gait cycle. Resultant force magnitude computed from measured three-dimensional force components obtained from the OrthoLoad database(Bergmann et al., 2014). The waveform exhibits the characteristic double-peak pattern associated with physiological walking. Source: Author´s own work (2026).

The predicted stress response, closely followed the temporal pattern of the applied in-vivo force, exhibiting peak alignment, during high-loading phases of the gait cycle, demonstrating monotonic and physically consistent load–response behaviour as shown in figure 4.15.

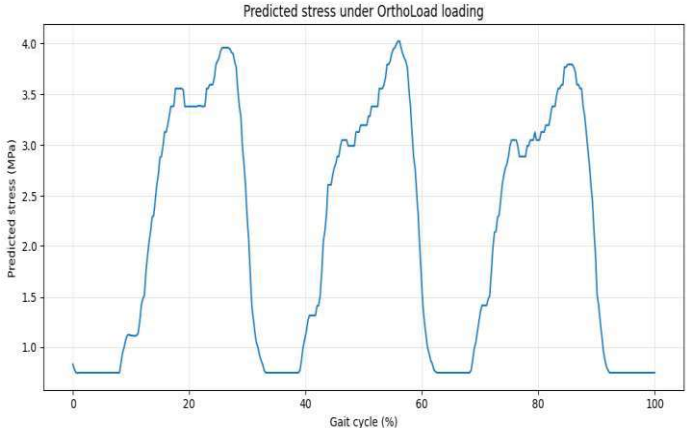


Figure 4.15. Predicted stress response under OrthoLoad loading. Predicted stress over a normalised gait cycle using in-vivo OrthoLoad forces as input. The stress response exhibits peak alignment with force maxima, indicating preservation of monotonic load–response behaviour under external loading conditions. Source: Author´s own work (2026).

The corresponding wear proxy, also demonstrated high values during force maxima, consistent with the proportional dependence defined by Archard (1953), as shown in figure 4.16.

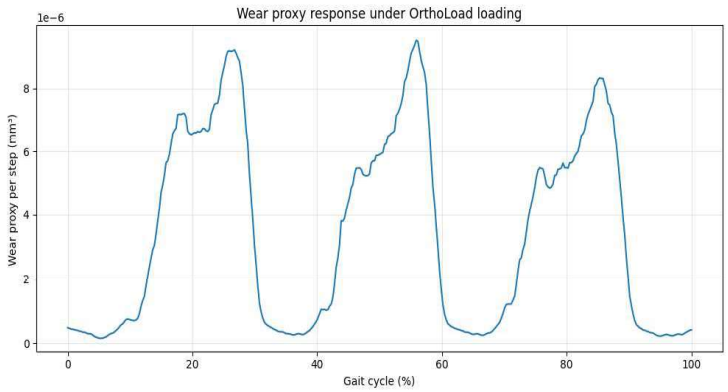


Figure 4.16. Wear proxy response under OrthoLoad loading. Wear proxy values computed using the hybrid AI–physics framework under OrthoLoad loading. Elevated wear during peak loading phases reflects the proportional dependence of wear on normal force as defined by Archard's law. Source: Author´s own work (2026).

These results indicate that the model preserves, physically consistent load–response relationships, when exposed to real measured forces, outside the synthetic training distribution. Also, it is important to know that it supports the external generalisation capability of the model.

4.4.4 Validation Layer 4: Multi-design robustness Assessment (Envelope Analysis)

To evaluate the stability of the model across implant design variability, an envelope-based robustness analysis, was performed under identical OrthoLoad in-vivo loading conditions. Ten implant configurations, were sampled from the synthetic design space, incorporating variation in geometric and material parameters, while maintaining the same external force input. This approach, enables assessment of predictive stability across the parameter space, rather than for a single representative configuration. For each design instance, predicted stress and wear responses were computed over the normalised gait cycle. The resulting stress envelope is presented as the median response with a 10–90% percentile band as shown in figure 4.17.

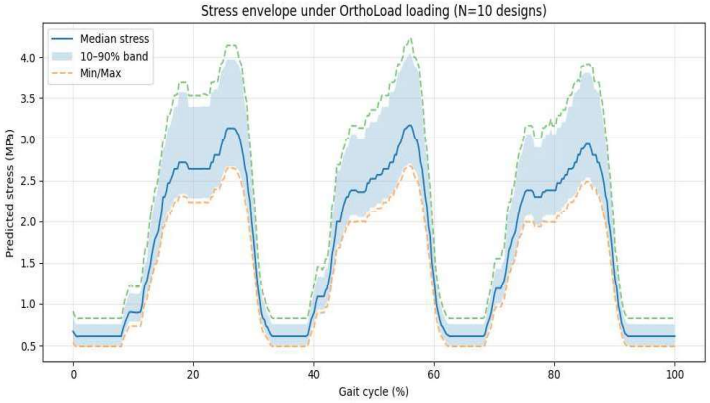


Figure 4.17. Median predicted stress over the normalised gait cycle with 10–90% percentile band for ten implant configurations. Source: Author´s own work (2026).

The resulting stress envelope is presented as the median response with 10–90% percentile band. While magnitude varies according to geometric and material properties, all configurations preserve the characteristic double-peak gait structure of physiological walking, demonstrating stable model behaviour across the design space. Similarly in figure 4.18, the wear envelope demonstrates proportional variation in predicted wear during peak loading phases, reflecting sensitivity to design parameters, while preserving the temporal gait structure.

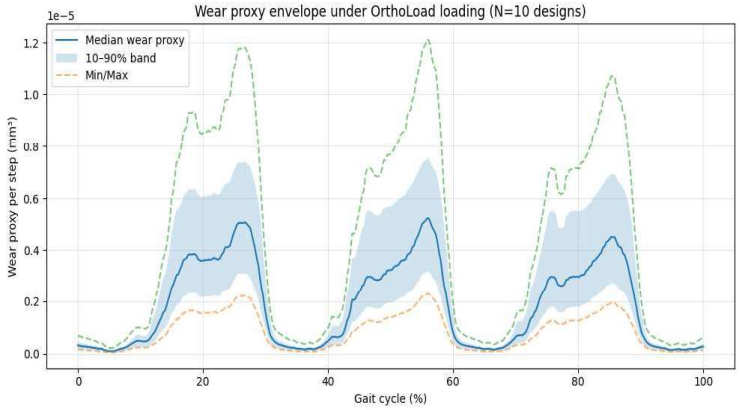


Figure 4.18. Wear proxy envelope across implant configurations under OrthoLoad loading. Predicted wear proxy over the gait cycle for ten implant configurations, presented as median response with 10–90% percentile band. Variability reflects design sensitivity while maintaining consistent temporal alignment with loading peaks, indicating robustness of the hybrid AI–physics framework. Source: Author´s own work (2026).

All configurations, preserved the characteristic double-peak temporal structure associated with physiological walking, consistent with the applied OrthoLoad waveform (Bergmann et al., 2014). While response magnitudes varied across configurations, reflecting expected sensitivity to thickness, stiffness, and contact-related parameters, no non-physical oscillations or instabilities were observed.

The envelope behaviour, confirms that the model, maintains monotonic load–response relationships, and temporal coherence, across the explored design domain. This robustness is essential, for digital screening applications, where comparative evaluation of multiple design candidates is required. Although envelope variability does not constitute optimisation or clinical validation, it demonstrates stable generalisation, within the sampled parameter space, and supports the reliability of the framework for parametric exploration, under physiologically realistic loading.

Chapter 5
Discussion

5.1 Interpretation of Results

5.1.1 Synthetic Dataset Behavior and Physical Consistency

The exploratory data analysis confirmed, that the synthetic dataset preserved expected biomechanical relationships. The strong positive correlation between axial load and stress ($r = 0.859$), reflects the fundamental contact mechanics behaviour, where stress increases proportionally with applied load, and decreases with contact area (Bartel et al., 1986). The strong relationship, between stress and deformation ($r = 0.819$), also, conforms with classical elastic strain theory (Nordin & Frankel, 2012).

The observed right-skewness in wear distribution, (skewness = 3.008), is consistent with the multiplicative structure of Archard's wear formulation (Archard, 1953). Since wear is proportional to the product of load and sliding distance, and inversely proportional to hardness, extreme parameter combinations naturally, generate disproportionately high wear values. The higher number of IQR outliers, for wear relative to stress and deformation, reflects this cumulative and nonlinear behaviour.

Overall, the dataset exhibits, statistical stability and physical plausibility, indicating that the synthetic generation process, did not introduce artificial distortions.

5.1.2 Machine Learning Performance for Stress and Deformation

The ensemble tree-based models, the Random Forest and Gradient Boosting, not only achieved high predictive accuracy for stress ($R^2 > 0.98$), but also, a strong performance for deformation ($R^2 \approx 0.95$). These results, indicate that the correlations between stress and deformation, as specified by parameter space, are highly learnable, using structured regression methods.

In comparison to the ANN, the enhanced performance of tree-based models, for deformation prediction, aligns with evidence that ensemble approaches, often surpass neural networks on structured tabular datasets (Grinsztajn et al., 2022). The Neural networks generally, require larger datasets, and careful architecture tuning, to achieve comparable generalisation (James et al., 2013).

The notably low R^2 (0.048) for ANN in deformation prediction suggests sensitivity to hyperparameter configuration or insufficient sample size relative to network complexity. Importantly, this result reinforces the need for model selection tailored to data structure rather than default reliance on deep learning approaches.

5.1.3 Wear Prediction Complexity

When compared to stress and deformation models, the wear prediction, demonstrated moderate explanatory power ($R^2 = 0.586$), which is significantly lower. This outcome is expected, given the hidden intricacy of tribological processes. Unlike stress, which depends primarily on load and contact area, wear depends on many interacting multiplicative variables including load, sliding distance, hardness, wear coefficient, and accumulated cycles.

It is important to note that tribological systems, exhibit variability and nonlinear accumulation behaviour, which may account for the moderate predictive performance of the model (V. Kumar et al., 2025). The wear model preserved monotonic relationships consistent with Archard's law, and sensitivity analysis confirmed expected parameter influence trends. Thus, while the model does not achieve high R^2 comparable to stress prediction, it remains suitable for screening-level assessment rather than precise lifetime estimation.

5.2 Implications for Orthopaedic Device Development

The results suggest that physics-informed synthetic data, combined with machine learning, can approximate biomechanical trends, without immediate reliance on computationally intensive finite element simulation. This approach, may support early-stage design exploration, by enabling rapid comparison of geometric and material configurations.

Such digital frameworks, align with broader digital transformation initiatives in healthcare engineering, where computational tools increasingly complement experimental workflows (Karniadakis et al., 2021). By providing trend-based screening prior to laboratory testing, this approach may reduce time-to-design iteration and associated resource expenditure. Furthermore, the ability to generate reproducible synthetic datasets addresses common data scarcity challenges in medical device research.

5.3 Validation Against ISO and In Vivo Data

Validation was structured to examine physical consistency, behavioural stability under gait loading, external generalisation using in-vivo forces, and robustness across implant design variability. Parametric sensitivity analysis, confirmed that predicted stress increased monotonically with axial load, consistent with classical contact mechanics principles (Bartel et al., 1986). Predicted deformation, on the other hand, decreased with increasing implant thickness, reflecting the expected stiffness–compliance relationship in elastic load-bearing components(Nordin & Frankel, 2012).

Furthermore, wear increased proportionally with cycle count, consistent with Archard's wear law, which defines wear volume as proportional to normal load and sliding distance (Archard, 1953). These findings, indicate that the model preserved, fundamental mechanical relationships, rather than learning false correlations.

Behavioural validation, using an ISO-informed gait waveform, demonstrated that predicted stress and wear responses , preserved the characteristic double-peak structure, observed during physiological walking, as reflected in ISO 14243 simulator standards (*ISO 14243-1*, 2009; *ISO 14243-3*, 2014).

External validation, using OrthoLoad in-vivo forces, further confirmed that the model generalised, to independent measured loading profiles (Bergmann et al., 2014).

Finally, envelope analysis across multiple implant configurations, demonstrated stable temporal behaviour, with magnitude variation attributable, to geometry and material differences. Collectively, these findings support the mechanical interpretability and robustness of the proposed digital framework.

5.4 Digital Screening and Equity in Resource-Constrained Settings

The proposed digital framework, may hold particular relevance for healthcare systems, operating under resource constraints. In many regions in the world, such as Africa, and Nigeria in particular, access to advanced wear simulators, high-performance computational infrastructure, and extensive experimental testing facilities, remains limited.

By enabling early-stage implant screening, using synthetic data and surrogate modelling, the framework reduces reliance on expensive laboratory validation, during preliminary design exploration. While regulatory approval, will always require formal physical testing, AI-assisted digital pre-screening, may lower initial research and development barriers, support local innovation ecosystems, and promote more sustainable, biomedical engineering practices.

In this context, digital surrogate modelling, represents not a replacement for traditional validation, but an enabling technology that broadens participation in orthopaedic device development.

5.5 Limitations

Despite encouraging validation results, several limitations must be acknowledged. First, the synthetic dataset, was generated using predefined parameter ranges, and simplified assumptions regarding contact behaviour and wear modelling. While ranges were informed by biomechanical literature and ISO standards, the synthetic generation process cannot fully replicate complex in-vivo tribological phenomena such as, cross-shear, lubrication regime transitions, or microstructural fatigue mechanisms.

Second, the surrogate framework relied primarily on scalar axial load magnitude rather than full multi-axis loading and kinematic waveforms specified in ISO 14243-1 and ISO 14243-3 (*ISO 14243-1*, 2009; *ISO 14243-3*, 2014). Although behavioural and external validation, demonstrated temporal consistency, full simulator replication was beyond the scope of the present work.

Third, the wear model was based on Archard's proportional wear relationship (Archard, 1953), which represents a simplified macroscopic approximation, rather than a comprehensive tribological model.

Finally, no direct experimental wear calibration, or clinical outcome data were incorporated. Therefore, the framework should be interpreted, as a digital screening and exploration tool, rather than a clinically validated predictive system.

5.6 Comparison with Existing Literature

Finite element–based wear simulations, remain the dominant computational approach, in implant biomechanics (Abdelgaied et al., 2022). While such models provide high spatial resolution of stress distributions, they are computationally demanding and often limited to a small number of design configurations.

Recent research has explored machine learning applications, in orthopaedic biomechanics; however, many studies focus primarily on predictive accuracy without layered validation against physical principles or in-vivo data.

The present work contributes by integrating synthetic data generation, supervised machine learning, physics-informed wear modelling, ISO-referenced behavioural validation, and external validation using OrthoLoad in-vivo measurements (Bergmann et al., 2014).

This approach, remains less extensively explored in the context of modular all-polymer tibial trays. This study contributes to bridging that gap by demonstrating feasibility of a unified digital screening framework.

5.7 Future Work

Future extensions could strengthen the framework, by incorporating full multi-axis ISO waveforms, including anterior–posterior displacement and tibial rotation components. Integration of flexion-angle-dependent contact modelling, would further enhance biomechanical realism. Experimental calibration against physical wear simulator data would allow quantitative benchmarking of predicted wear volumes against ISO 14243 test results.

From a modelling perspective, advanced generative models such as, variational autoencoders or diffusion-based synthetic data generators may expand parameter diversity.

Additionally, extension to other daily activities, including stair ascent and descent using OrthoLoad datasets, would improve activity generalisation. Ultimately, integration into clinical decision-support or regulatory pre-screening pipelines would represent a significant advancement toward practical digital orthopaedic workflows.

Conclusion

Summary of Key Findings

This thesis developed and validated a quantitative, physics-informed, data-driven digital framework for predicting biomechanical stress, deformation, and wear in modular all-polymer knee trays, manufactured from PEEK-OPTIMA ^{TM}. By integrating synthetic data generation, supervised machine learning regression, and hybrid Archard-based wear modelling, the framework demonstrates, the feasibility of early-stage digital screening, in orthopaedic implant development. A synthetic dataset of 8000 multidimensional design samples, was generated using Latin Hypercube Sampling, to ensure uniform parameter coverage. Exploratory data analysis, confirmed statistical stability, and preservation of basic biomechanical relationships, such as, strong association, between axial load and stress, and cumulative wear dependence on loading cycles.

The ensemble tree-based machine learning models, achieved high predictive accuracy for stress ($R^2 > 0.98$), and strong performance for deformation ($R^2 \approx 0.95$), while neural network performance was less consistent. Wear prediction demonstrated moderate explanatory power ($R^2 \approx 0.59$), reflecting the inherent nonlinear and cumulative nature of tribological processes.

Validation against ISO 14243 loading standards and multi-design OrthoLoad in vivo envelopes confirmed that synthetic loading conditions remained within both standardised laboratory and physiological ranges while the envelope analysis across multiple implant configurations, showed stable temporal behaviours that support the mechanical interpretability and robustness of the validated digital framework.

Achievement of Objectives

The primary aim of this study was to develop and validate a quantitative, physics-informed digital framework capable of generating synthetic biomechanical data and predicting stress, deformation, and wear in modular all-polymer PEEK-OPTIMA ^{TM} tibial trays. This aim has been achieved. All stated objectives were fulfilled:

1. A reproducible synthetic data generation pipeline was implemented using Latin Hypercube Sampling.

2. Machine learning models were trained and evaluated for stress and deformation prediction.
3. Archard's wear equation was integrated within a hybrid computational framework.
4. Validation was conducted against ISO 14243 standards and OrthoLoad in vivo datasets.
5. Ethical and reproducibility considerations were addressed through synthetic data usage and transparent documentation. The alignment between methodological design and reported results demonstrates internal coherence of the research.

Contributions to Digital Transformation in Healthcare

This study contributes to digital orthopaedics by demonstrating that physics-informed synthetic data combined with machine learning can approximate biomechanical trends without reliance on immediate finite element simulation or laboratory wear testing. The key contributions include:

i) A unified computational workflow integrating sampling, regression, and wear modelling.
ii) Comparative evaluation of ensemble and neural network approaches for biomechanical regression.
iii) Demonstration of dual validation against standardised and in vivo loading envelopes.
iv) A reproducible and ethically compliant synthetic modelling framework. These findings support the broader integration of AI-assisted design screening tools within medical device development pipelines.

Final Remarks

While not a substitute for regulatory testing or clinical validation, the proposed framework provides a structured, interpretable, and computationally efficient approach for early-stage biomechanical exploration. The moderate wear prediction performance, highlights the inherent complexity of tribological processes, and underscores the importance of future experimental calibration. Overall, this work has established a foundation for physics-informed digital screening of polymer-based knee implant components, and contributed to the evolving landscape of orthopaedic device development workflows, through a digital transformation approach.

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Appendix A: A Comparison Of ISO 14243 VS The Key Selected Synthetic Data Ranges For The Model Training.

ISO 14243 parameters were used as reference for magnitude and gait-style validation, while the synthetic dataset uses simplified scalar loading and motion proxies to support data-driven surrogate modeling. Table below: gives a comparison of ISO 14243 vs the key selected synthetic data ranges for the model training. This table A.1 complements the table 3.1 in methodology and the further description in the google colab code.

Table A.1: A comparison of ISO 14243 vs the key selected synthetic data ranges for the model training.

Category	ISO 14243 typical ranges	key selected synthetic data ranges	Justification/Inclusion criteria
Axial load	168–2600 N	500–3000 N	Slightly higher max (3000) and higher min (500), "broader envelope than ISO."
Cycles	5,000,000	100,000 – 5,000,000	ISO full test plus shorter early-stage screening.
Frequency	1 Hz	not modeled	No time/thermal effects claim. Model is cycle-based, so frequency isn't required.
Flexion/ Extension	0–58°	not included	Important for "ISO-style kinematics" but contact area was used instead. Directly relates to contact pressure: stress ≈ load / area. Keeps the model simple and stable. Works well with OrthoLoad resultant forces. Instead contact area was used.
AP motion / force	0 –5.2 mm (disp) or −265 to +110 N	sliding 0.5–5 mm/cycle	Close proxy to AP displacement magnitude (good for simplified wear). But not the same as ISO waveform.
Tibial rotation	−5.7° to +1.9° or torque −1 to +6 Nm	not included	Only for ISO kinematics.
Test medium/temp	serum ~20 g/L @ 37°C	not modeled	Only needed for modelling lubrication/temperature-dependent wear.

Appendix B: Sampling Code Snippets

```
    def sample_inputs_lhs(n=8000, seed=42):
        """
          Latin Hypercube Sampling (LHS) for implant/material/loading
inputs.
       Continuous variables via LHS; cycles sampled log-uniform (integer).
        """
        rng = np.random.default_rng(seed)

        param_ranges = {
            "thickness_mm": (6.0, 14.0),
            "curvature_radius_mm": (20.0, 60.0),
            "contact_area_mm2": (600.0, 1200.0),
            "E_GPa": (3.0, 5.0),
            "nu": (0.35, 0.42),
            "hardness_MPa": (150.0, 300.0),
            "axial_load_N": (500.0, 3000.0),
            "sliding_mm_per_cycle": (0.5, 5.0),
        }

        names = list(param_ranges.keys())
        lower = [param_ranges[n][0] for n in names]
        upper = [param_ranges[n][1] for n in names]

        sampler = qmc.LatinHypercube(d=len(names), seed=seed)
        unit = sampler.random(n=n)
        scaled = qmc.scale(unit, lower, upper)
        df = pd.DataFrame(scaled, columns=names)

        # cycles: log-uniform for wide range realism
        cycles_min, cycles_max = 100_000, 5_000_000
        log_min, log_max = np.log10(cycles_min), np.log10(cycles_max)
          df["cycles"] = (10 ** (log_min + (log_max - log_min) *
rng.random(n))).astype(int)

        # engineered feature
        df["stiffness_proxy"] = df["E_GPa"] / df["thickness_mm"]

        return df

    X_raw = sample_inputs_lhs(n=8000, seed=SEED)
    X_raw.to_csv("data/lhs_input_parameters.csv", index=False)

    print("Generated LHS inputs ✓")
    X_raw.head()
```

Appendix C: Model Hyperparameters & Summary EDA

Random Forest:

- n_estimators = 300
- max_depth = 12
- min_samples_split = 2

Gradient Boosting:

- n_estimators = 300
- learning_rate = 0.05
- max_depth = 4

ANN_MLP:

- Hidden layers = (64, 32)
- Activation = ReLU
- Solver = Adam
- Max iterations = 500

EDA SUMMARY — Synthetic Knee Tray Dataset (LHS)

- Dataset shape: 8000 rows × 13 columns
- Missing values: None detected
- Top absolute correlations (|r|):
- axial_load_N vs stress_MPa: 0.859
- stiffness_proxy vs thickness_mm: 0.834
- deformation_mm vs stress_MPa: 0.819
- axial_load_N vs deformation_mm: 0.709
- wear_mm3 vs cycles: 0.708
- stiffness_proxy vs E_GPa: 0.490
- thickness_mm vs deformation_mm: 0.424
- contact_area_mm2 vs stress_MPa: 0.419

- Skewness note: wear_mm3 skew = 3.008 (right-skew expected for cumulative wear)
- IQR outlier counts
  :• stress_MPa: 41,
  • deformation_mm: 203,
  • wear_mm3: 776

Appendix D: Data Card for Synthetic Knee Tray Dataset (LHS) (Digital-Only)

1. About the Dataset

This synthetic Knee Tray Dataset (LHS) is associated with the Master's thesis: "A Hybrid AI–Physics Framework for Synthetic Biomechanical Modelling and Wear Prediction in Modular All-Polymer Knee Trays (PEEK-OPTIMA™): A Digital Transformation Approach in Orthopaedic Data science"

Date created: 2026-02-04

Creator(s): Obasi Chinedu Chamberlin & Dr. Mitha Rachel Jose

Organisation(s): ISCTE – University Institute of Lisbon, Portugal, Laurea University of Applied Sciences, Finland and Aristotle University of Thessaloniki, Greece.

Rights-holder(s): Copyright 2026 ManagiDiTH

Contact Emails: Chinedu_Obasi@iscte-iul.pt, mitha.jose@laurea.fi

Summary: This dataset is entirely synthetic and to be used to Train ML models to predict stress, deformation, and estimate wear for modular all-polymer knee tray proxies. It represents a parametric design space for modular all-polymer knee trays (PEEK-OPTIMA™) and includes physics-informed proxy labels for stress and deformation, plus Archard-based wear proxies. The dataset was designed specifically for the development and evaluation of machine learning regression models within the digital workflow proposed in this research.

Generation Method: Latin Hypercube Sampling (LHS) for continuous parameters; cycles sampled log-uniform (integer).

Composition: The dataset contains 8,000 samples and 13 variables, including input parameters and predicted biomechanical outputs.

Features: ['thickness_mm', 'curvature_radius_mm', 'contact_area_mm2', 'E_GPa', 'nu', 'hardness_MPa', 'axial_load_N', 'cycles', 'sliding_mm_per_cycle', 'stiffness_proxy']

Targets: stress_MPa, deformation_mm, wear_mm3

Intended Use: Early-stage digital screening and educational/research use. Not intended for regulatory decisions or direct clinical claims.

Limitations: Labels are proxies, not FEA or experimental measurements**,** simplified material/contact assumptions and wear units are proxy-scale; not calibrated to a specific simulator results.

Data Pre-Processing and Validation: Basic exploratory data analysis (EDA) was conducted to assess the statistical properties of the generated dataset. The analysis confirmed: No missing values in the dataset, Logical correlations between key mechanical variables (e.g., load–stress relationship), expected right-skew behaviour in cumulative wear values, acceptable statistical variability across the sampled parameter ranges. Outliers identified in deformation and wear variables were retained because they represent plausible extreme design conditions within the sampled parameter space.

2. Terms of Use:

Copyright 2026 ManagiDiTH. This dataset is to be licensed under a Creative Commons Attribution 4.0 International Licence: https://creativecommons.org/licenses/by/4.0/.

3. Project and Funding Information:

ManagiDiTH – Master's Degree of Managing Digital Transformation in the Health Sector project under EC grant agreement 101083896.Co-Funded by the European Union.
Dates: 2023 - 2026

3. Data Availability:

The synthetic dataset generated for this research is included in the thesis supplementary materials.

Additional implementation details, including data generation scripts and model training procedures, are provided in the appendices and accompanying code repository.

Interested parties should check the contact emails.

4. Ethical and Privacy Considerations:

The dataset does not contain any patient data, personal information, or clinical records.

All values were generated synthetically through statistical sampling and mechanical modelling. Therefore, the dataset complies with General Data Protection Regulation (GDPR) requirements and does not pose privacy risks. The use of synthetic data in this research also supports ethical AI practices by avoiding the use of sensitive clinical datasets while enabling methodological experimentation.

Appendix E: Model Card for Machine Learning Models Used in Biomechanical Prediction (Digital-Only)

1. About the Models

These machine learning models associated are with the Master's thesis: "A Hybrid AI–Physics Framework for Synthetic Biomechanical Modelling and Wear Prediction in Modular All-Polymer Knee Trays (PEEK-OPTIMA™): A Digital Transformation Approach in Orthopaedic Data science"

Date created: 2026-02-04

Creator(s): Obasi Chinedu Chamberlin & Dr. Mitha Rachel Jose

Organisation(s): ISCTE – University Institute of Lisbon, Portugal, Laurea University of Applied Sciences, Finland and Aristotle University of Thessaloniki, Greece.

Rights-holder(s): Copyright 2026 ManagiDiTH

Contact: Chinedu_Obasi@iscte-iul.pt , mitha.jose@laurea.fi

Summary: "This study applied machine learning regression models to predict biomechanical responses of all-polymer knee implant trays manufactured from PEEK-OPTIMA™. The models were designed to estimate two primary mechanical outputs: Implant stress (MPa) and Implant deformation (mm). A hybrid modelling approach was also used to estimate implant wear, where machine learning predictions of stress were integrated with Archard's wear equation. Three machine learning algorithms were evaluated: Random Forest, Gradient Boosting and Artificial Neural Network. The goal was to compare model performance and identify the most reliable model for predicting biomechanical behaviour within the synthetic design space".

Models compared: Random Forest, Gradient Boosting, and ANN.

Best stress model: GB | Metrics stored in artifacts/model_metrics.json

Best deformation model: GB | Metrics stored in artifacts/model_metrics.json

Wear model: Archard baseline + hybrid stress-modulated k (artifacts/wear_metrics.json)

Training Data: Synthetic dataset generated as described in the Data Card.

Training Procedure: The machine learning models were trained using the synthetic dataset consisting of 8,000 samples. The dataset was split into: Training set: 80% of samples and Testing set: 20% of samples. Model performance was evaluated using common regression

metrics: Root Mean Square Error (RMSE), Mean Absolute Error (MAE) and Coefficient of Determination (R^2). These metrics were used to evaluate prediction accuracy and model generalisation.

Model Hyperparameters: Basic hyperparameter tuning was conducted to optimise model performance.

Hyperparameter configuration: Models and Key Hyperparameters:

Random Forest: n_estimators, max_depth

Gradient Boosting: learning_rate, n_estimators

ANN_MLP: hidden_layer_sizes, activation function

The tuning process was performed using grid-based experimentation to identify parameter combinations that produced stable prediction performance.

Intended Use: For exploratory implant design analysis, educational research in digital biomechanics and demonstrating hybrid AI–physics modelling approaches. They are not intended for clinical decision-making or regulatory validation without further experimental testing.

Limitations: The models were trained on synthetic data rather than experimental implant data. Simplified mechanical relationships were used to estimate stress and deformation. The models do not capture complex joint behaviours such as, lubrication, multi-directional loading, or biological responses. Despite these limitations, the models demonstrate the feasibility of combining machine learning with physics-based wear estimation to support early-stage implant design exploration.

2. Terms of Use

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3. Project and Funding Information

ManagiDiTH – Master's Degree of Managing Digital Transformation in the Health Sector project under EC grant agreement 101083896. Co-Funded by the European Union.

Dates: 2023 – 2026.

4. Model Availability

Please interested parties should check the contact emails.

5. Ethical and Privacy Considerations:

- No patient-identifiable data
- Reproducible pipeline with stored configuration and fixed random seeds.