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REVIEW ARTICALE

COMPUTATIONAL EVALUATION OF THE BIOMECHANICAL AND BIOCOMPATIBILITY BEHAVIOUR OF BIOMATERIALS FOR ORAL REHABILITATION

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ABSTRACT

Background: Recent advancements in computer simulations present promising alternatives for investigating the biomechanical performance, degradation, and biocompatibility of dental materials, especially polymethyl methacrylate (PMMA), zirconia, and titanium-based structures. The aim of this review was to examine the biomechanical behaviour, molecular interactions, degradation trends, and biocompatibility of different dental biomaterials employed in oral rehabilitation utilising advanced computational techniques.

Materials and Methods: Finite Element Analysis (FEA) is used to simulate the distribution of stress inside the prosthetic restoration, underlying implant and peri-implant tissues, utilising 3D models of the jawbone, abutments, and restorations. Molecular dynamics simulations alongside in silico toxicity screening tools are valuable for evaluating the degradation behaviour and possible biological interactions of PMMA and other dental polymers under various simulated conditions. Models for protein-ligand docking can be employed to explore interactions between biomaterial monomers and target receptors that are pertinent to biocompatibility and toxicity.

Results: Computational modelling can successfully pinpoint abnormal stress zones linked to implant failure and anticipated stress-strain responses under functional loads. At the molecular level, simulations may demonstrate structural changes in PMMA induced by environmental stress, including chain deterioration and loss of flexibility under elevated humidity and thermal stress. In silico toxicity assessments highlight potential reactive sites within polymer structures and provide predictive insights into their biocompatibility. Interaction modelling verified either favourable or undesirable binding affinities with biological receptors, depending on the composition of the material.

Conclusion: Computational methodologies offer a cost-effective, scalable, and highly detailed strategy for both biomechanical and biological evaluation of dental biomaterials. This multiscale modelling approach addresses the limitations of conventional empirical techniques by allowing the prediction of clinical outcomes and biocompatibility at both structural and molecular levels. The study lays the groundwork for a safer selection and design of materials in prosthodontics and implantology, emphasizing the importance of incorporating computational methods in future biomaterial research.

Keywords: Dental biomaterials, computational modelling, PMMA, finite element analysis, in silico toxicity, molecular dynamics, oral rehabilitation, implant-supported prosthesis, biocompatibility.

INTRODUCTION

It is consistently difficult to eliminate subjectivism when evaluating the characteristics of prosthodontic materials due to the uncertainty in the assessment criteria within dental research. The use of computational techniques for studying dental biomaterials has become increasingly popular, primarily driven by scientific progress and advancements in computer technology. Over the last five years, there has been a growing interest in this area of dental biomaterials and its research developments. Numerous new biomaterials have been introduced in the field of dentistry; however, their behaviour and effects on the structures of the oral cavity and the overall body are still not thoroughly understood. Notable examples include titanium (Ti) and its alloys, yttria-stabilised zirconia (YTZP), zirconium-reinforced lithium silicate, lithium-disilicate-reinforced glass ceramics, and acrylic resins with improved mechanical properties [1,2]. Alongside these innovative materials, glass fibres and nanoparticles show considerable potential for reinforcing other foundational materials and resin structures. Significantly, the mechanical properties of polymethyl methacrylate (PMMA) denture base materials can be enhanced through the implementation of a hybrid system, hybrid fillers, or a combination of both as a new reinforcement strategy. Research in this field primarily takes place in vitro, but there is an increasing demand for innovative approaches that implement computational techniques [3,4].

Traditional empirical methods for assessing materials have inherent limitations when it comes to revealing the complex atomic and electronic interactions that govern material behavior[5]. These standard methods often neglect the subtleties of the electronic structure, which impedes accurate examinations of bonding mechanisms, charge transfer processes, and the impact of defects or impurities. Conversely, computational methods offer a detailed view of the electronic framework of materials, enabling a comprehensive analysis of electron distribution in dental implant materials [6,7].

Nevertheless, existing research has frequently fallen short, lacking a molecular-level understanding of the interactions between biomaterials and biological systems. Furthermore, there is a dearth of thorough evaluations of the safety profiles of different prosthetic and dental implant materials using in silico methods. This has resulted in a significant gap in the literature regarding the detailed molecular examination of biocompatibility and toxicity of dental biomaterials. Furthermore, there has been an insufficient number of in-depth studies on the behavior of various biomaterials used in oral rehabilitation through computational modeling [5,7]. The aim of this review is to systematically explore the biomechanical properties, molecular interactions, degradation behavior, and biocompatibility of different dental biomaterials used in oral rehabilitation by utilizing advanced computational techniques.

Stress simulation

Computer modelling has become a powerful and effective method for quantifying the forces applied at specific moments during biomechanical evaluations. It is a valuable tool for forecasting stress distributions within prosthetic structures, peri-implant areas, and the interfaces of implant-supported frameworks. Advanced computational methods can reveal abnormal stress patterns that lead to implant failures, concentrating on the primary stress combinations at specific points of interest [8,9].

The incorporation of computerised technology enables a comprehensive analysis of biological tissues and synthetic materials' stress-strain behaviours, thus aiding the geometric design of complex anatomical structures while linking them to their mechanical characteristics. The computed stresses can be consistently compared among simulated models, helping to determine if proposed oral rehabilitation methods may be susceptible to mechanical failure under loading conditions [10,11].

Utilising digital technologies to examine biomechanics provides a straightforward method for validating stress distributions related to implants. Given the complex geometric features in prosthetic constructions, dental implants, and the surrounding bone systems, computer simulations are increasingly acknowledged as the best way to assess these components [8,11].

A significant challenge faced by many researchers is the financial strain and intricacies associated with experimental testing apparatus. In this regard, computerised approaches offer notable benefits, such as improved time efficiency, ease of use, and cost savings [12].

As a crucial tool for assessing and simulating the detailed biomechanical aspects of surgical situations, computer simulation offers a thorough and reliable framework for examining the mechanical properties of complex structures. Especially in implantology, computer simulation has developed into a significant and promising tool for biomechanical analysis. It allows researchers to investigate stress distributions in different implant components and surrounding osseous tissues, critically analysing the biomechanical properties of implants and predicting their clinical results. Computer simulation offers manifold benefits over traditional physical model approaches, enhancing the precision and efficiency of biomechanical research [8-11]. Components of the dental implant system for finite element analysis are shown in Figure 1 and 2 [13-15].

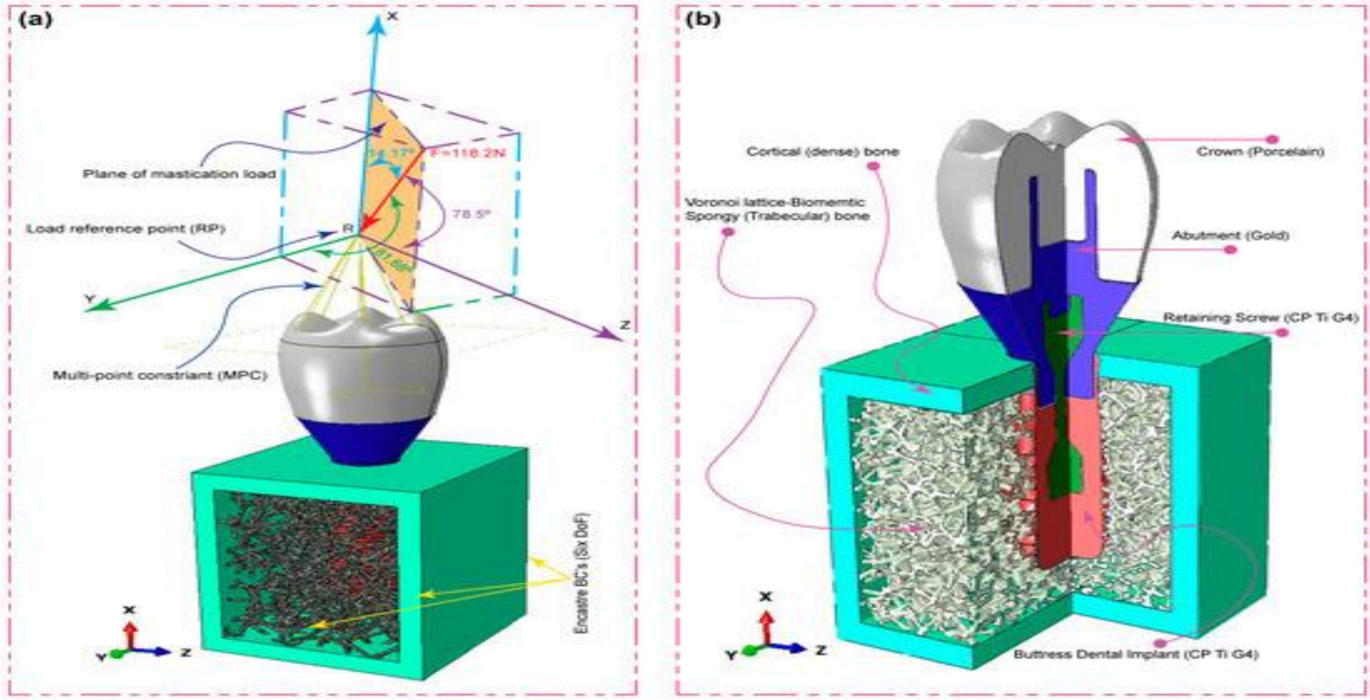

Figure 1. Components of the dental implant system, including the following: (a) application of dynamic explicit oblique loading at the load reference point with the MPC constraint, (b) 3D model components designed for finite element analysis [13].

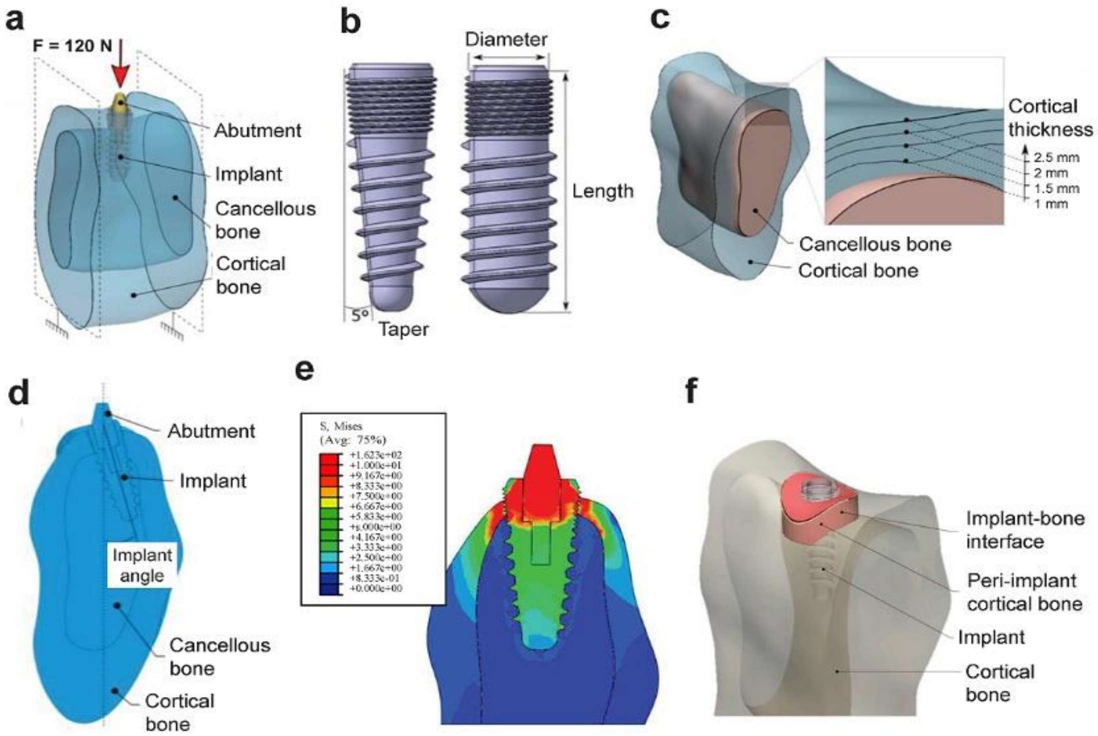

Figure 2. (a) Finite element models. boundary conditions and loading (b), implant design (c), mandibular section showing various cortical thicknesses (d), configuration of the implant in the bone in the vestibulo-lingual plane (e), Von Mises stress distribution (f), a diagram of the cortical bone peri-implant area [14,15].

Biomolecular simulation

The application of advanced computational technologies enables a nuanced understanding of molecular interactions and dynamic behaviors arising from the interfacial interactions among various biomaterials. A range of in silico tools can facilitate toxicity assessments, allowing for the prediction of potential toxic elements or compounds inherent in dental materials. These modern analytical methodologies serve as critical resources for evaluating the biocompatibility and toxicity profiles of dental materials, particularly addressing the limitations of traditional biological compatibility assessment methods that often fail to provide molecular-level insights into interactions between these materials and biological systems [12,16].

The advent of sophisticated in silico techniques permits researchers to delve deeper into molecular interactions between dental materials and biological tissues, systematically addressing complex questions that have remained unanswered regarding these interactions. Rapid in silico screening methods are pivotal in identifying potential hazards associated with dental materials, thereby influencing more informed material selection decisions for interim prosthetic restorations following tooth loss. Through these computational approaches, we aim to elucidate the behavior of materials at the macromolecular interaction level within biological contexts, enabling a more predictive understanding of the biocompatibility and toxicity of PMMA-based dental materials in a systematic and cost-effective manner [16-18].

Computational simulation techniques facilitate the study of atomic and molecular dynamics over time, allowing for an in-depth observation of material behaviors at an atomic scale. This capability is instrumental for investigating complex systems, such as polymers, where traditional experimental methodologies may be constrained by limitations in temporal or spatial resolution [18-21]. Additionally, advancements in 3D printing technologies, notably fused deposition modeling (FDM) and stereolithography (SLA), have enabled precise control over the microstructural and mechanical properties of PMMA. The tailoring of these characteristics offers significant potential for the evolution of dental materials and other applications [22-25].

However, despite the advantages of PMMA, concerns regarding its environmental degradation, particularly under varying temperature and humidity conditions, persist. Therefore, it is crucial to elucidate the relationship between these environmental factors and the mechanical behavior of 3D-printed PMMA to enhance its durability and reliability [26].

Computational simulations have provided critical insights into the atomic-level molecular scenarios governing the degradation of PMMA chains. For an extended period, real-time observations of PMMA dental materials at an atomic resolution have been lacking. This methodological framework can be employed to investigate structural changes, molecular interactions, and degradation processes, providing a deeper understanding of material responses under diverse environmental stimuli [18-26]. PMMA chains are presented in Figure 3.

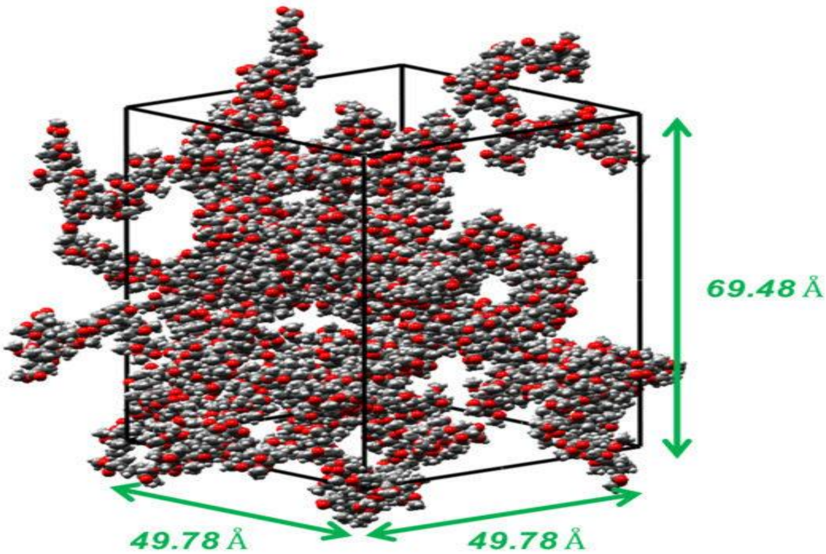

Figure 3. Amorphous cell composed of 50 PMMA chains of length 16 [27].

Virtual Testing of Dental Material Behaviour

For the assessment of the load distribution on the bone, implant, and prosthetic construction, a virtual geometric model of the jaw, implant, abutment, and prosthetic construction is acquired. The 3D model is divided into small elements, showing how the load is distributed across different areas. For the assessment of the biocompatibility and toxicity of the polymeric materials, first, the receptors responsible for biocompatibility are selected as targets. The 3D structure of the selected receptors is modelled using computer software. The 3D structure of the selected biomaterials is also modelled. The interaction between the selected dental biomaterials and the receptor is modelled computationally. The behaviour of the materials is evaluated dynamically under simulated oral cavity conditions. Computer software predicts the potential toxicity of different biomaterials or their components. For the biodegradation assessment, PMMA chains are created using digital modelling methods. Humidity is simulated by adding water (20%–100% humidity). Temperature variation is simulated within the 300 K – 600 K range. After the simulation begins, changes in the polymeric material are monitored. Under different simulated conditions, the material's flexibility, strength, and structural formation are calculated for each case [16,17,27-29].

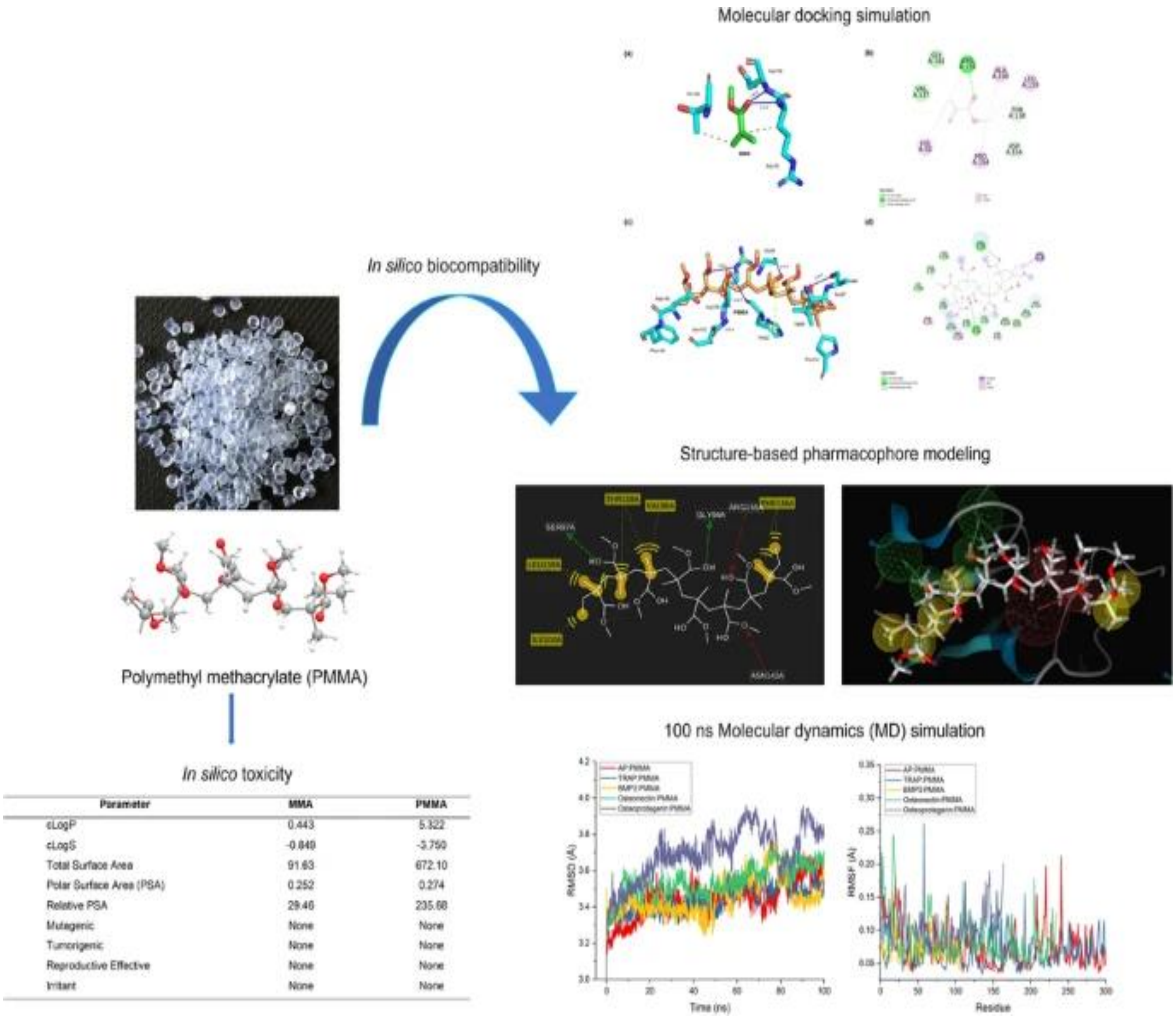

Figure 4. In silico assessment of biocompatibility and toxicity: molecular docking and dynamics simulation of PMMA-based dental materials for interim prosthetic restorations [16].

DISCUSSION

This study illustrates the effectiveness and flexibility of computational simulation methods in the comprehensive evaluation of dental biomaterials. These techniques enable thorough assessments of mechanical properties, biocompatibility, toxicity, and environmental durability, overcoming the limitations associated with traditional experimental approaches [16,17].

Employing finite element analysis (FEA) to model stress distribution in prosthetic frameworks supported by implants provided insights that are often unattainable via in vitro methods. By creating geometric models of anatomically precise structures, such as the jawbone, implant, abutment, and prosthetic elements, our simulation allowed for localised visualisation of stress concentration and distribution. Such analyses are particularly important for identifying regions vulnerable to mechanical failure due to excessive loads, particularly in peri-implant areas. The results reinforce the increasing belief that computer simulation is not only a feasible substitute for physical prototyping but also a superior technique for preliminary evaluation of implant design and material choice [8-11, 30-32].

An important characteristic of this work is its investigation of biomaterial biocompatibility at the molecular level. By modelling the 3D structures of receptor proteins and biomaterials and simulating their interactions in silico, we can explore the potential for unfavourable biological responses. This complex approach presents predictive insights into possible inflammatory, toxic, or immunogenic responses. Traditional assays seldom capture atomic-level interactions; thus, this method addresses an essential knowledge gap. Additionally, this approach facilitates high-throughput toxicity screening, allowing for the fast elimination of inappropriate candidates early in the planning process [16-18, 33-35].

Simulating environmental factors, such as varying humidity and temperature, provided essential insights into the structural durability of polymer-based dental materials like PMMA. The molecular dynamics simulations showed that increased temperature and moisture levels considerably affect the flexibility, integrity, and chain stability of PMMA. These results are consistent with existing literature that highlights the vulnerability of PMMA vulnerability to hydrolytic and thermal degradation. Furthermore, quantifying degradation impacts under specific environmental conditions allows informed decisions regarding material suitability in various clinical settings, such as for patients with xerostomia or high oral acidity [16-18, 36].

Using computational data to optimise 3D printing parameters is a promising direction for personalising dental prosthetics. The ability to adjust microstructural features through additive manufacturing methods, such as fused deposition modelling (FDM) and stereolithography (SLA), allows for tailoring mechanical properties to satisfy specific clinical requirements. When guided by molecular simulations, this initiative can create more durable, biocompatible, and environmentally robust prosthetic devices [24,25].

Although this study highlights the advantages of computational simulations, it also has limitations. The precision of the simulation models relies on the quality of the input data, which includes molecular geometries and boundary conditions. Moreover, while in silico tools provide quick and cost-effective assessments, their predictions must eventually be verified through clinical trials to ensure their reliability for real-world application. Future investigations should focus on combining machine learning algorithms to enhance the predictive precision of these models and broaden their use to a broader array of innovative biomaterials.

CONCLUSION

This review highlights the important contribution of computational simulation in comprehensively evaluating dental biomaterials. By employing advanced modelling methods, it is possible to virtually evaluate the biomechanical properties, molecular interactions, biodegradation characteristics, and biocompatibility of materials commonly used in oral rehabilitation. The ability to simulate stress distribution within the prosthetic restoration, implant and peri-implant tissues presents crucial insights into mechanical stability and possible points of failure. Additionally, the molecular-level analysis of material–biological interactions provides predictive insights into toxicity and compatibility, which addresses the shortcomings of traditional empirical approaches. Various environmental factors can lead to the biodegradation of different biomaterials, especially PMMA, highlighting the necessity for material optimisation specific to those conditions. Combining 3D printing and computational modelling presents new opportunities for developing personalised prosthetic treatment. This review reinforces the importance of in silico methodologies as valuable and economical tools for advancing dental material science. Future studies should prioritise validating these models through clinical trials and broadening the research scope to encompass a broader range of biomaterials and patient-specific factors.

DECLARATION

Ethical Approval

Not applicable

Informed consent statement

Not applicable

Consent for publication:

Not applicable

Availability of data and materials

The data supporting this study's findings are available from the corresponding author upon reasonable request.

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