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Extensive Iterative Finite Element Analysis of Molar Uprighting with the Introduction of a Novel Method for Estimating Clinical Treatment Time

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Abstract: The aim of this study was to analyze the biomechanical effects of a conventional molar uprighting spring on a mesially tilted mandibular second molar through a novel iterative finite element (FE) approach in order to estimate clinical treatment duration. A new model was developed utilizing data from previous canine retraction experimental studies to aid in correlating each individual FE iteration with its real-time value. Another model consisting of a 30° mesially titled mandibular second molar and a conventional molar uprighting spring was developed to evaluate kinetic and kinematic responses. The iterative FE simulation of the treatment was then carried out. The molar uprighting simulation was completed in 180 iterations, which was equivalent to almost 12 weeks of clinical treatment time. The average stress-normalized bone remodeling velocity was found to be ~0.9 µm/(KPa·day). During the simulation, the spring initially produced a 15 N·mm (~1530 g·mm) counterclockwise moment responsible for molar uprighting. The mandibular second molar showed 3.75 mm of distal movement, 2.15 mm of vertical extrusion, and a 22° counterclockwise rotation at the end of the treatment. This study provides a foundation for the future estimation of biomechanical responses as a function of treatment time in various orthodontic applications using iterative FE simulations.

Keywords: mesially tilted molar; conventional uprighting spring; orthodontics; biomechanics; tooth movement rate; bone remodeling velocity; iterative finite element analysis



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1. Introduction

One of the most common conditions which can be seen in the orthodontic clinic is the presence of a mesially tilted mandibular second molar occupying the space of the adjacent missing first molar [1]. Numerous oral health issues can result from a patient's tilted molar, particularly if prosthetic rehabilitation is intended. These include angular bone loss, inflammation, and an apparent pocket at the mesial surface of the tilted molar, all of which are symptoms of worsening periodontal health [2].

To prevent functional and anatomical disruptions, the loss of a permanent first molar should be addressed with a prosthetic replacement or orthodontic space closure [3]. In order to create an acceptable path of insertion for a fixed prosthesis when we have limited space for a pontic, it is necessary to over-prepare the mesial side of the tilted molar, which

could result in pulp exposure and improper loading on the tooth. Hence, orthodontic molar uprighting is the treatment of choice to facilitate creating proper space for the prosthetic replacement of a missing permanent first molar while maintaining or improving the periodontal environment in that area [4].

There are multiple appliances that can be utilized for molar uprighting [1,2,5]. One of the classical ways to upright a tilted molar is the use of a conventional molar uprighting spring, which was introduced by Burstone in 1966. This method is a segmental approach, where the spring is manually made by creating a loop in a heavy rectangular stainless-steel wire and hooking it on the anchorage teeth segment while engaging the tilted molar for uprighting [6,7].

Finite element (FE) analysis has been proven as a reliable method for investigating the biomechanical effect of different orthodontic appliances on the periodontal ligament (PDL) behavior and other related structures [8]. Although FE analysis is a key numerical tool in dental biomechanical research [9–11], only a handful of studies have focused on molar uprighting springs [12–15]. Furthermore, numerous FE studies have been performed to predict orthodontic tooth movement; nevertheless, only few have addressed the analysis of bone remodeling related to long-term orthodontic tooth movement [16–19].

There have been previous attempts to determine the tooth movement rate and iteration time for orthodontic applications using FE analysis [20–22]. However, the correlation and conversion of this iteration time into real clinical time in order to estimate orthodontic treatment duration remains an area to be explored [23].

Thus, the study aims to investigate the kinetic and kinematic responses of a mesially tilted mandibular second molar and the associated anchoring segment to an activated conventional uprighting spring through a novel FE approach for estimating clinical treatment duration. The null hypothesis of this study was that the iterative finite element simulation of molar uprighting would not produce clinically realistic estimates of tooth movement, treatment duration, or stress-mediated bone remodeling behavior.

2. Materials and Methods

To simulate long-term molar uprighting and estimate its clinical treatment duration, two models were developed and executed in parallel. Model 1 represented the canine retraction simulation using vertical loop mechanics and was developed to establish a time calibration framework. Model 2 corresponded to the molar uprighting simulation using a conventional uprighting spring and was implemented as an iterative FE model to capture progressive biomechanical responses. Experimental data on tooth velocity from canine retraction studies were combined with FE simulations to derive the bone remodeling velocity as a function of mean stress in the PDL. This relationship was then applied to Model 2, permitting the conversion of each simulation iteration into its corresponding clinical time duration, enabling the interpretation of long-term molar uprighting biomechanics in clinically meaningful units.

2.1. Model 1: Canine Retraction Simulation

The first computer-assisted design (CAD) model was developed based on previous studies that assessed canine translation velocity under continuous, constant forces [24,25]. These studies, which bridge clinical observations with experimental data, are essential for establishing a novel FE modeling technique capable of estimating real clinical time for a single simulation iteration, and thus the total treatment duration.

For that purpose, a two-dimensional (2D) CAD representation of the maxillary canine was reconstructed, with 0.2 mm of PDL thickness and alveolar bone surrounding the tooth using SolidWorks® software (Version 2022, Dassault Systèmes, Vélizy-Villacoublay, France).

The incorporated appliances included a standard edgewise bracket of 0.022-inch slot size bonded on the maxillary canine and a segmental 0.019 × 0.025-inch stainless steel wire shaped to resemble a vertical open loop with a height of 13 mm which engaged the canine on the distal side (Figure 1). Using Abaqus/Standard software (Version 2022, Dassault Systèmes, Vélizy-Villacoublay, France), constant forces ranging from 0 to 800 cN with an increment of 10 cN, were applied to translate the canine distally and carry out the simulation process.

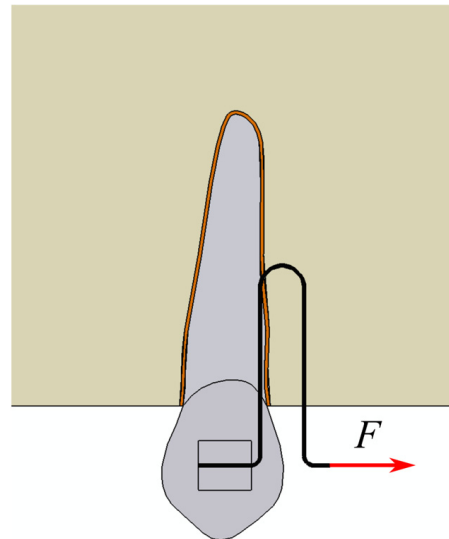


Figure 1. Finite element (FE) representation of Model 1 for the canine retraction using vertical loop mechanics. The mesh distribution illustrates local refinement around the periodontal ligament (PDL) to ensure the accuracy and convergence of the results. A distal force ‘F’ is applied through a looped spring to translate the maxillary canine, simulating experimental retraction conditions for time calibration.

Experimental studies [24,25] provided clinical data on canine translation velocity under constant forces of up to 1600 cN. In the current FE simulation, constant forces ranging from 50 to 800 cN were applied, as this range was sufficient to establish the correlation. The simulation outcomes included tooth displacements and PDL deformations, which were used to calculate the real-time duration of each numerical step. The overall workflow for obtaining this calibration is outlined in Figure 2. By calculating the bone remodeling velocity and average mean stress in the PDL, a correlation was established and can be seen in Figure 3. This relationship enabled the translation of stress levels into remodeling velocities and served as the basis for the time calibration applied in the molar uprighting model. Additionally, Figure 3 illustrates the original relationship between tooth displacement velocity and applied force [24].

The process summarized above presents a framework for relating the bone remodeling velocity to average mean stress in the PDL, allowing its application across a range of orthodontic loading conditions. This relationship can be leveraged to estimate the equivalent real clinical time for any applied force at any simulation iteration, ultimately enabling the prediction of both total orthodontic treatment duration and tooth movement rate using FE modeling. To authors’ knowledge, this study is the first to introduce such an approach.

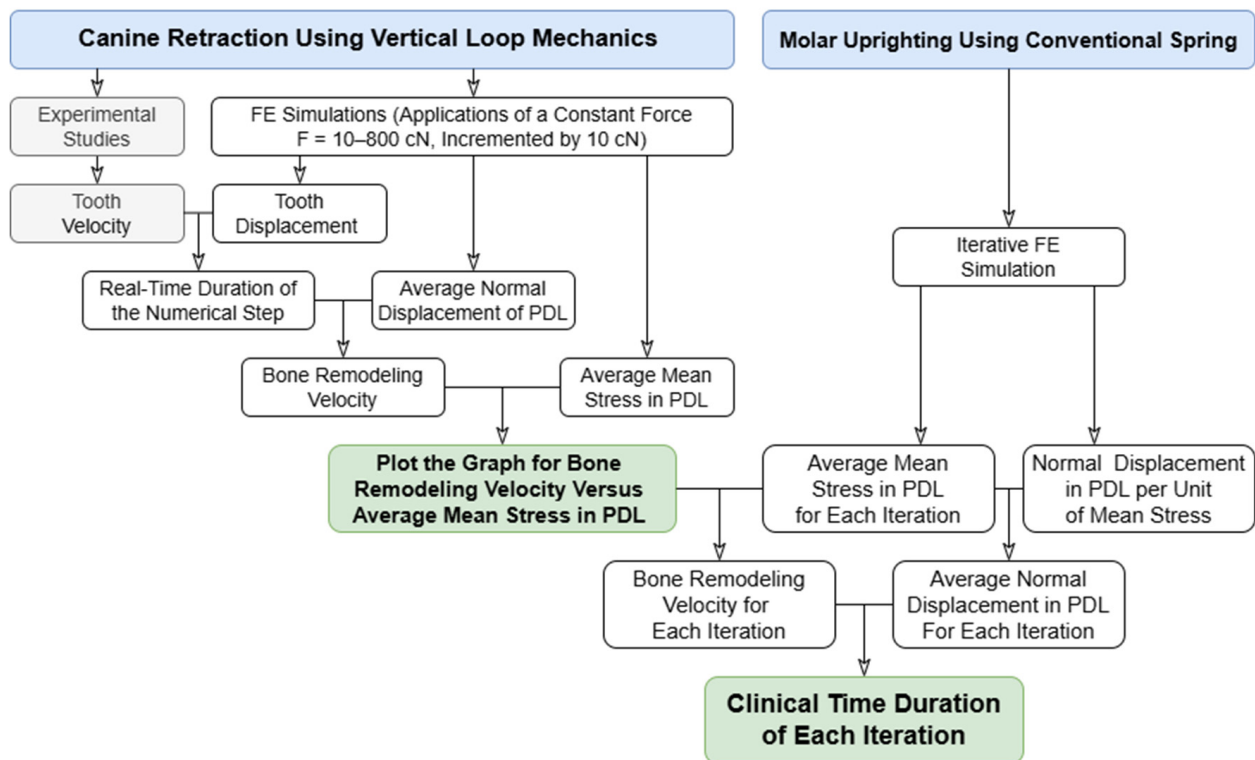


Figure 2. Flowchart illustrating the calibration process used to convert FE simulation iterations into real clinical treatment time. The left pathway represents canine retraction using vertical loop mechanics, combining experimental data and simulations to derive a relationship between bone remodeling velocity and average mean PDL stress. This relationship was then applied to the molar uprighting simulation (right pathway) to compute the clinical time duration of each iteration.

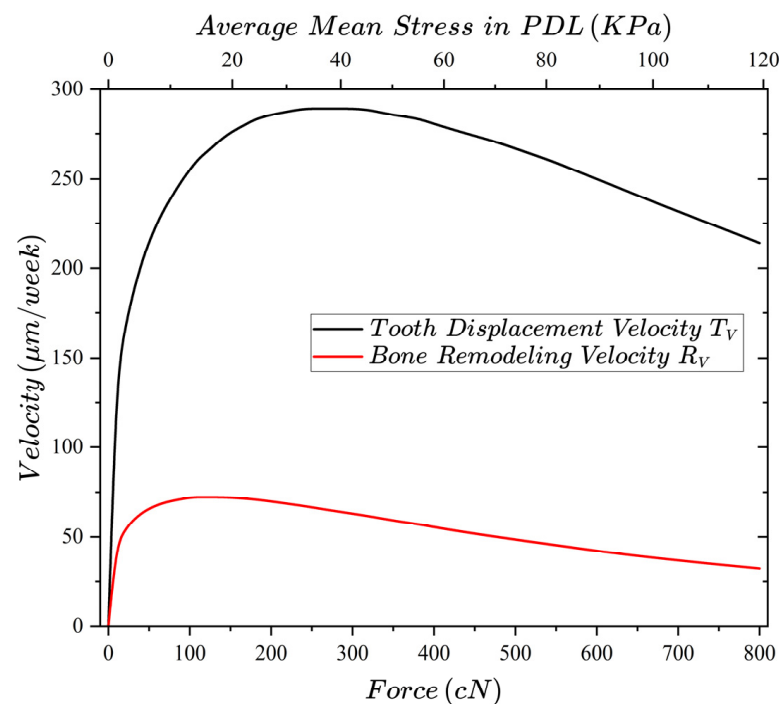


Figure 3. Tooth displacement velocity and bone remodeling velocity plotted as functions of the applied retraction force and the corresponding computed average mean stress in the PDL. The black curve represents tooth displacement velocity during canine retraction based on experimental data from previous studies [24]. The red curve shows the bone remodeling velocity derived from the current study using Model 1.

2.2. Model 2: Molar Uprighting Simulation

A second CAD model was also developed using SolidWorks® software. Initially, a three-dimensional (3D) model of the mandible's right posterior teeth segment was reconstructed from a computed tomography (CT) scan image, obtained from the DICOM-image repository provided via osirix database "<https://www.osirix-viewer.com> (accessed on 20 November 2023)". The 3D CAD model was then converted into a 2D CAD representation by extracting its edges along a central plane intersecting the middle of the teeth. The periodontal ligament (PDL) was assigned a uniform thickness of 0.2 mm, an average value widely supported by anatomical literature [26]. While this simplification does not capture local anatomical variations—such as root concavities or patient-specific PDL irregularities—it provided a stable and practical framework for the iterative simulation process. Similarly, the dental geometry preserved the essential morphological features relevant to sagittal-plane movement, though finer anatomical details were not included. These modeling choices were intentional, as the study focused on capturing the overall biomechanical trends driving molar uprighting, rather than resolving localized stress concentrations, while still ensuring reliable results for the proposed iteration-to-time correlation method.

The characteristics of this model were adapted from the previous literature [13]. The model consisted of a mandibular second molar tilted by 30° mesially, with the mandibular canine and first and second premolars acting as the anchorage teeth. The incorporated appliances included standard edgewise brackets of 0.022-inch slot size bonded to the anchorage teeth, a 4 mm wide edgewise molar buccal tube, and a segmental 0.016 × 0.016-inch stainless steel wire connecting the anchorage teeth. In addition to a conventional molar uprighting spring made of 0.016 × 0.016-inch stainless steel wire, with a 2 mm diameter helical loop and a long lever arm with a length of 22 mm. This long lever arm was projected anteriorly to lie passively 12 mm gingival to the anchorage wire between the first and second premolars, and was activated when raised and hooked onto the anchorage wire. The spring's short lever arm, as defined in this context, represented the arm engaging the molar buccal tube slot and was assumed cinched at the distal end of the buccal tube to prevent any possible sliding of the wire (Figure 4).

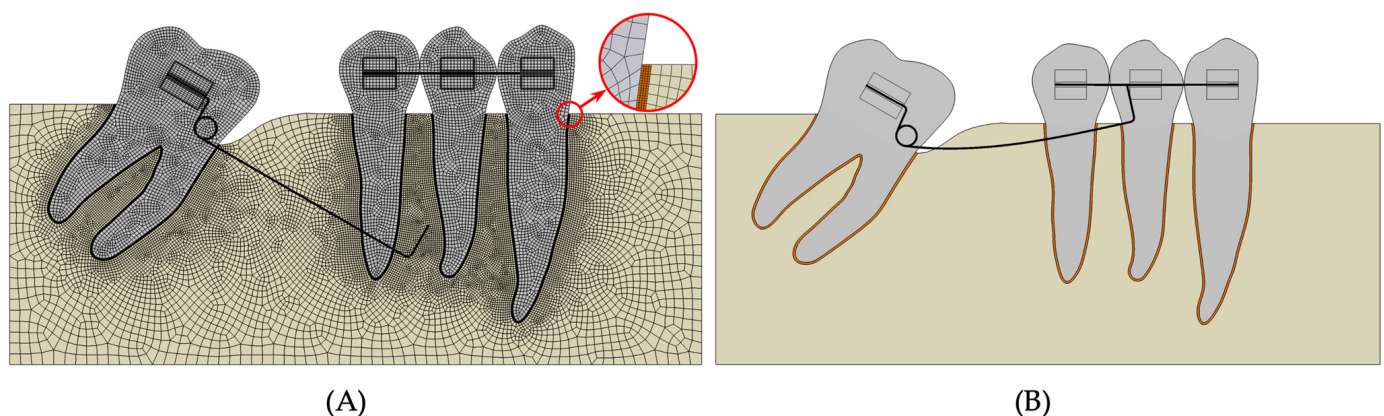


Figure 4. Finite element (FE) representation of Model 2 for molar uprighting using a conventional uprighting spring. (A) FE mesh of the initial configuration before spring activation; (B) CAD representation of the configuration after spring activation.

A 2D plane stress mesh was generated in Abaqus/Standard software using exclusively linear quadrilateral elements (CPS4R) with reduced integration. A total of 461 two-node linear beam elements (B21) were used to model the uprighting spring as a slender 0.016" × 0.016" stainless steel component. The use of quadratic beam elements did not provide any gain in terms of stress capture with a significant increase in computation time.

To better capture contact forces, a very fine mesh (0.05 mm) was applied to the portion of the wire inserted into the bracket. The contact between the wire and bracket was modeled using a friction coefficient of 0.28, as reported in previous studies [27,28].

The mesh was also locally refined around the PDL and root surfaces to improve accuracy in regions with high stress gradients. A total of 4279 CPS4R elements were generated to model the molar PDL. The use of the Medial Axis Algorithm for mesh control enabled a symmetrical distribution of elements along both the bone–PDL and root–PDL interfaces. This configuration is essential to ensure that the displacement of an element in contact with the root is transmitted, along an identical normal vector, to a single corresponding element on the bone interface. To assess mesh independence, simulations were repeated using progressively finer meshes. Displacement and stress values varied by less than 2% between successive refinements, confirming acceptable convergence at a mesh size of 0.05 mm. This resolution also ensures at least four elements across the thickness of the PDL, which helps mitigate the hourglass effects commonly associated with reduced integration elements [29].

As the geometry of the bone changes at each iteration, a Python (Version 2.7) script integrated into the simulation workflow automatically detects the surfaces in contact with the various PDLs and applies a finer mesh (0.1 mm) to these regions, with gradual coarsening toward the outer boundaries of the bone. As a result, up to 12,000 elements were generated within the bone domain. As for boundary conditions, the mesial and distal borders of the alveolar bone domain were fixed to prevent rigid-body motion, as the model was truncated at those locations to reduce computational cost while preserving mechanical stability.

The treatment simulation was carried out using Abaqus/Standard software. It began at the starting point of conventional uprighting spring activation and was completed when the equilibrium of forces was reached and the spring was considered no longer active. Contact between the brackets, molar buccal tube, and the uprighting spring generated teeth movements along with the gradual uprighting of the tilted molar.

This simulation was performed under the assumption that orthodontic tooth movement is directly correlated with initial tooth displacement [30], according to the bone remodeling algorithm proposed in the previous literature for simulating long-term orthodontic tooth movement [16]. The process started with the application of orthodontic force, inducing initial tooth displacement, which is reflected in the deformation of the PDL. In the next step, the outer surface of the PDL is repositioned to restore its original form and maintain its uniform thickness of 0.2 mm. Consequently, the geometry of the PDL is updated and the bone is remodeled based on the amount of PDL displacement. In this manner, the alveolar bone remodeling and long-term orthodontic tooth movement are simulated and executed in cycles or as an iterative process by the computer software and continues until the tilted molar is appropriately uprighted or the corrective forces dissipate, reaching the equilibrium state (Figure 5).

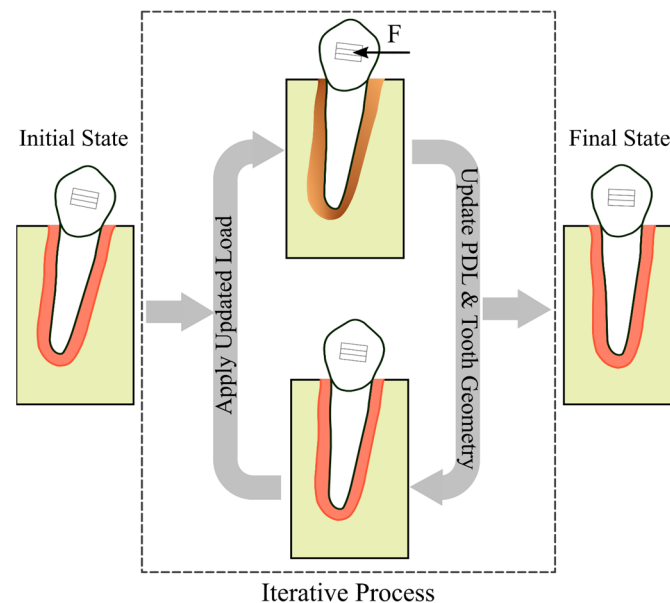


Figure 5. Iterative process for simulating long-term orthodontic tooth movement. At each iteration, the applied force ‘F’ produces PDL displacement, which drives bone remodeling and updates the tooth–PDL–bone geometry. The process continues until the corrective forces dissipate and equilibrium is reached.

2.3. Material Properties and Boundary Conditions

The mechanical properties of structures involved in both Model 1 and Model 2 were derived from previous literature [22] and can be seen in Table 1. All the models’ constituents were considered as linear, elastic, homogeneous, and isotropic materials, except for the brackets and molar buccal tube which were considered as rigid materials. Tie contact was assumed between the PDL–bone and PDL–root interface. Surface to surface contact was assumed between the brackets, molar buccal tube, and wires. The superior surface of the maxilla and the inferior surface of the mandible were both fixed in Model 1 and Model 2, respectively.

Table 1. Mechanical properties of the structures involved in both models.

Material	Young’s Modulus (MPa)	Poisson’s Ratio (ν)
Bone	3000	0.3
PDL	0.84	0.46
Teeth (Root/Dentin)	20,000	0.3
Teeth (Crown/Enamel)	70,000	0.3
Stainless Steel	200,000	0.3

3. Results

3.1. Estimation of Treatment Duration and Real Clinical Time

The distribution of the normal displacement and mean stress along the PDL profile of the second molar can be seen in Figure 6. The PDL’s normal displacement U_N almost followed the same pattern as the corresponding mean stress σ_M in the associated PDL element. The ratio of normal displacement to the mean stress U_N/σ_M along a normalized path characterizing the PDL–root interface, was labeled as D_{σ_M} and computed over 180 iterations of molar uprighting. The ratio resulted in $D_{\sigma_M} \approx 0.41 \mu\text{m/KPa}$, and was almost consistent throughout the treatment simulation; this can be demonstrated in the plotted curves for the first and last iterations.

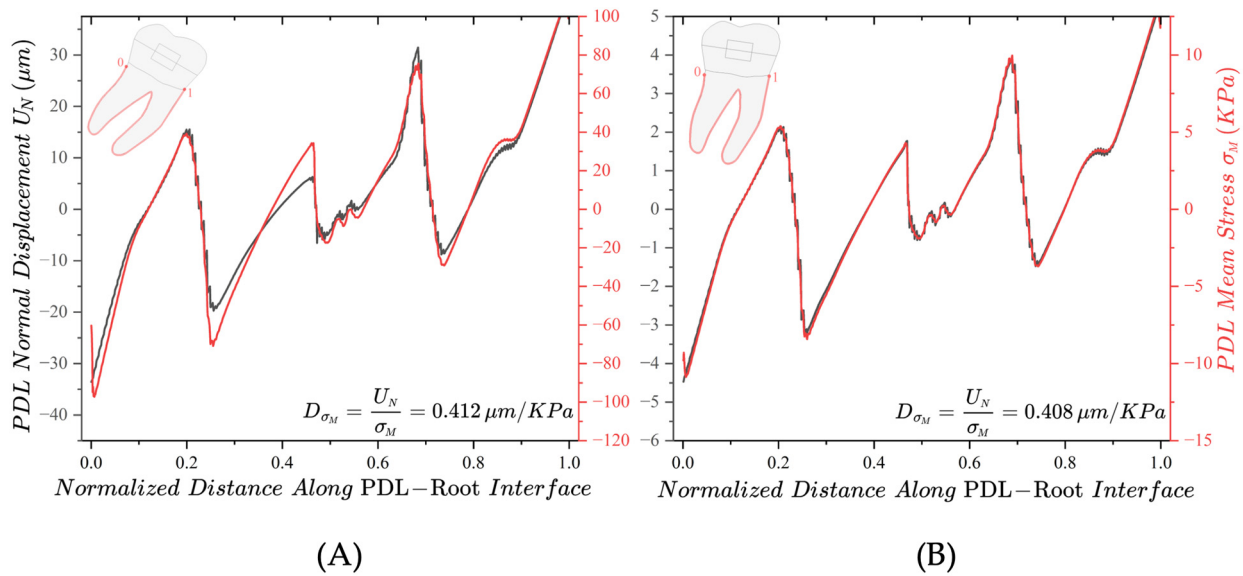


Figure 6. Distribution of normal displacement (U_N , black curve) and mean stress (σ_M , red curve) along the PDL-root interface of the second molar. (A) At the beginning of treatment (first iteration). (B) At the end of treatment (last iteration). The stress-displacement (D_{σ_M}) remains approximately constant at $\sim 0.41 \mu\text{m}/\text{KPa}$ across the interface, indicating a consistent mechanical response during the simulation.

Figure 7 presents the average mean stress in the PDL for each iteration of the molar uprighting simulation (black curve, left y-axis). This stress data was correlated with the bone remodeling velocity (red curve, right y-axis), using the relationship previously established and plotted in Figure 3, as detailed in the methodology section.

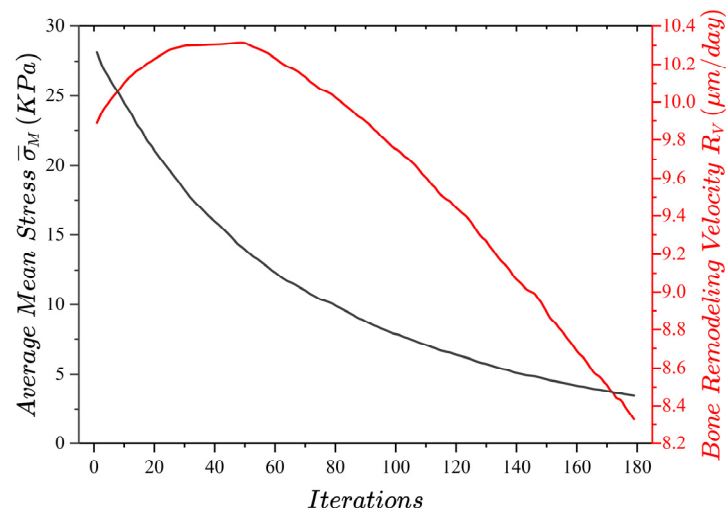


Figure 7. Evolution of the average mean stress $\bar{\sigma}_M$ in the PDL (black curve, left y-axis) and the corresponding bone remodeling velocity R_v (red curve, right y-axis) throughout the uprighting procedure, plotted as a function of finite element iterations.

Using the average mean stress $\bar{\sigma}_M$ and bone remodeling velocity R_v obtained at each iteration in Figure 7, and the corresponding normal displacement in the PDL $\bar{U}_N$ is calculated by multiplying $\bar{\sigma}_M$ by the stress-displacement ratio D_{σ_M} . The duration of each iteration T is then determined by dividing $\bar{U}_N$ by the remodeling velocity R_v , providing a real-time equivalent for that simulation iteration. This time increment is then added to the total cumulated treatment time T_{cum} , as illustrated in the flowchart in Figure 8. The process continues iteratively until the uprighting objective is achieved.

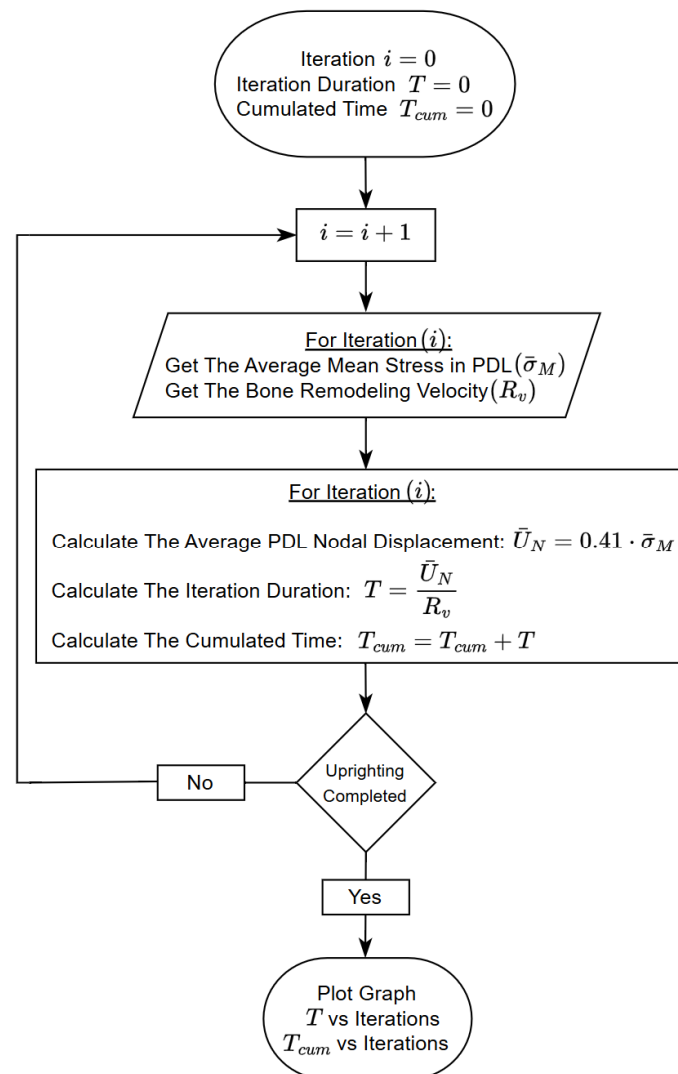


Figure 8. Flowchart outlining the iterative simulation process for time calibration. At each step, the average PDL stress and bone remodeling velocity are used to compute the normal displacement and iteration duration, which are cumulatively added until the uprighting goal is achieved.

The iterative framework outlined in the flowchart (Figure 8) enables the computation of both the duration of each simulation iteration and the corresponding accumulation of treatment time. As shown in the graph below (Figure 9), this process generates the evolution of iteration duration (black curve) and the total cumulated clinical time (red curve) throughout the uprighting simulation. As the uprighting progresses, the iteration duration decreases due to the gradual reduction in mechanical stimulus and remodeling activity, where the first iteration was the longest, lasting approximately 1.17 days, while the final iteration was the shortest, lasting around 0.18 days. The red curve (right y-axis) shows the cumulative clinical time, which increases nonlinearly and reaches approximately 12 weeks by the 180th iteration.

Based on the time-calibrated framework shown in Figures 8 and 9, the evolution of average mean stress in the PDL from Figure 7 can be interpreted in terms of clinical treatment time. The highest average mean stress value was approximately 28 KPa at the beginning of treatment and gradually decreased throughout the simulation. It dropped to around 8.8 KPa by iteration 90, which was equivalent to ~8 weeks of clinical duration, and reached approximately 3.5 KPa by the end of treatment simulation. In contrast, the bone remodeling velocity reached and maintained its peak values of ~10.3 $\mu\text{m}/\text{day}$ between

iterations 30 and 50, corresponding roughly to weeks 4 through 6 of the clinical duration. This plateau reflects the most active phase of tooth movement, which occurred when the average mean stress in the PDL was around the range of 14 and 18 KPa, after which both the mechanical stimulus and biological response progressively diminish as the uprighting process reaches its final stages. The computed average stress-normalized bone remodeling velocity over the 12-week treatment period was approximately $0.9 \mu\text{m}/(\text{KPa}\cdot\text{day})$.

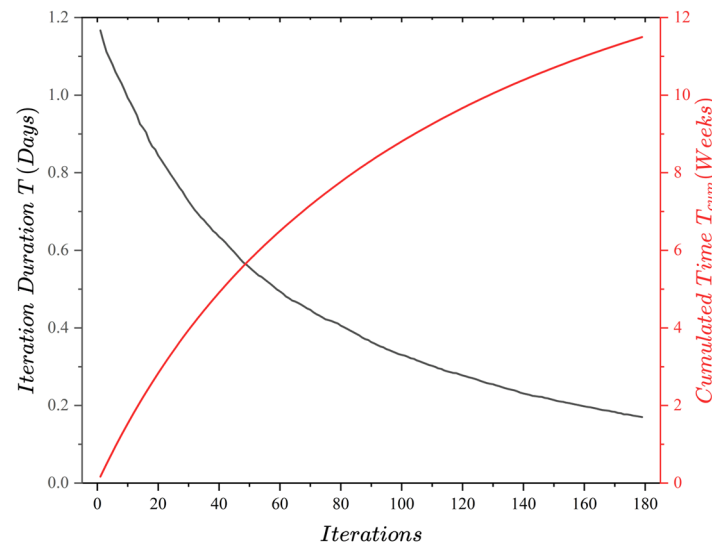


Figure 9. Calculated iteration duration in days (black curve, left y-axis) and corresponding cumulative clinical time in weeks (red curve, right y-axis), throughout the molar uprighting simulation.

3.2. Biomechanics of Molar Uprighting Using a Conventional Uprighting Spring

With the clinical duration of each simulation iteration now established, the biomechanical results for the molar uprighting process when using a conventional uprighting spring are expressed in terms of both clinical time and iteration number. Figure 10 displays the changes in the mandibular second molar position. Throughout the uprighting process, the molar showed approximately 3.75 mm of distal movement, 2.15 mm of vertical extrusion, and a 22° counterclockwise rotation. Throughout the simulation, the molar exhibited a steady biomechanical response, with distal movement and vertical extrusion progressing at average rates of approximately 0.31 mm/week and 0.18 mm/week, respectively, while counterclockwise rotation advanced at an average rate of $\sim 1.83^\circ$ per week.

According to the current study's calculations, the center of rotation (C_{Rot}) of the second molar was located approximately at the midpoint of the internal surface of the distal root, as shown in Figure 11. During molar uprighting, the C_{Rot} exhibited a slight shift occlusally of approximately 0.34 mm, while remaining nearly stable in the mesio-distal direction. This variation was minimal and nearly unnoticeable in Figure 11, which illustrates the C_{Rot} position at the first and last iterations.

The anchorage unit, consisting of the mandibular canine, first premolar, and second premolar, exhibited progressive vertical intrusion throughout the treatment simulation. As illustrated in Figure 12, the second premolar experienced the greatest intrusion, reaching approximately 0.37 mm by the end of the treatment. The first premolar followed with a total intrusion of around 0.30 mm, while the canine showed the least intrusion at approximately 0.21 mm. The rate of displacement appeared nearly constant across all anchorage teeth, falling within the range of 0.02–0.03 mm per week.

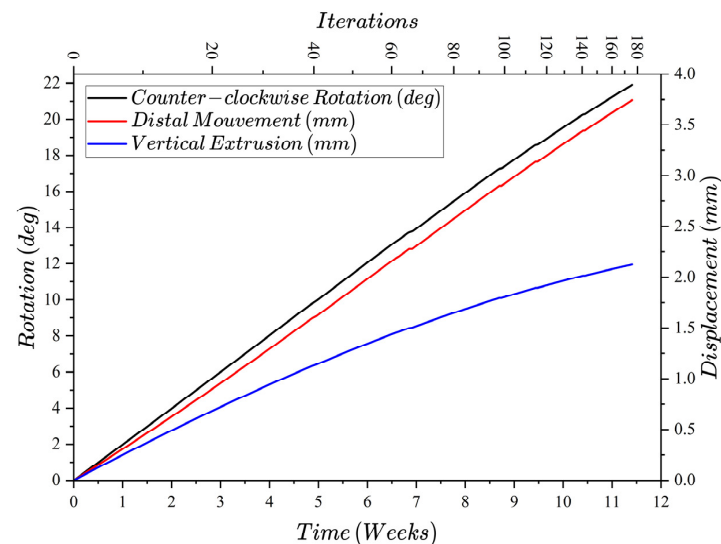


Figure 10. Molar distal movement, vertical extrusion, and counterclockwise rotation plotted over clinical treatment time (bottom x-axis) and corresponding simulation iterations (top x-axis). The curves illustrate the progressive tooth movement achieved throughout the 12-week molar uprighting process when using a conventional uprighting spring, with all movements occurring at an almost constant rate.

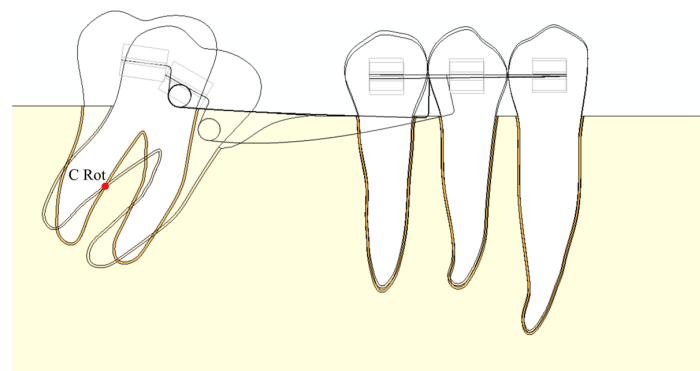


Figure 11. Estimated center of rotation (C_{Rot}) of the second molar during the uprighting process. The red dot indicates the C_{Rot} location, shown between the superimposed positions of the first and last iterations.

When analyzing the forces acting on the mandibular second molar in Figure 13, the graph presents the evolution of the uprighting moment at the buccal tube slot, the extrusion force, and the length of the spring's short lever arm. Here, the short lever arm is defined as the distance between the resultant upward mesial and downward distal contact forces applied at the opposing corners of the buccal tube slot. At the beginning of the treatment simulation, the spring generated a counterclockwise uprighting moment of approximately 15 N·mm (~1530 g·mm) and an extrusive force of 0.6 N (~61 g) acting on the molar. This extrusion resulted from the mesial contact force, applied to the upper corner of the buccal tube, being larger than the opposing distal force. As the molar uprighted over time, both the moment and extrusion force decreased steadily, reaching approximately 2.5 N·mm (~255 g·mm) and 0.09 N (~9 g), respectively, by the end of the treatment simulation. Insets A and B of Figure 13 highlight changes in the dimensions of the spring's short lever arm throughout the simulation. Initially, the effective lever arm length was 3.25 mm, defined by the distance separating the two resultant contact forces between the spring and the buccal tube slot. As uprighting progressed, these contact points shifted laterally toward the slot's outer edges. By the final iteration, the center of the distal force had moved closer to the lower distal

edge of the slot, increasing the effective short lever arm length to 3.96 mm, all without any wire sliding, but solely due to the reduction in bending deformation experienced by the spring wire as the molar uprighted. This shift reflects significant changes in load transfer dynamics as the mechanical system adapted during the simulation.

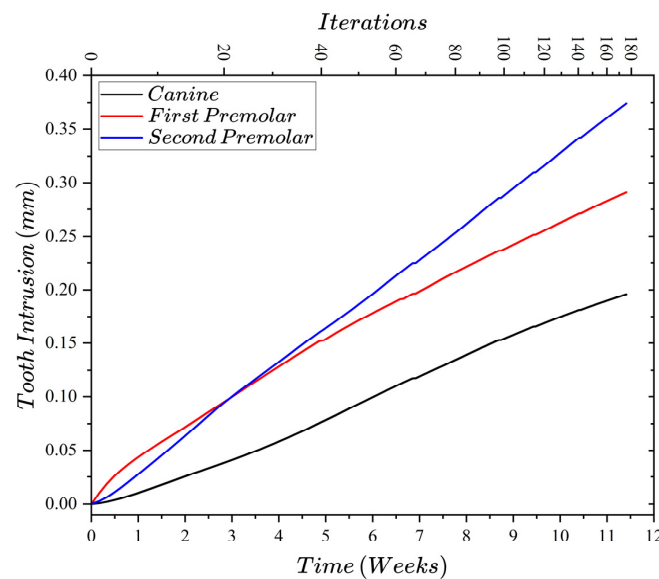


Figure 12. Vertical intrusion of anchorage teeth throughout the treatment simulation. All three teeth showed an almost constant rate of intrusion over the 12-week period.

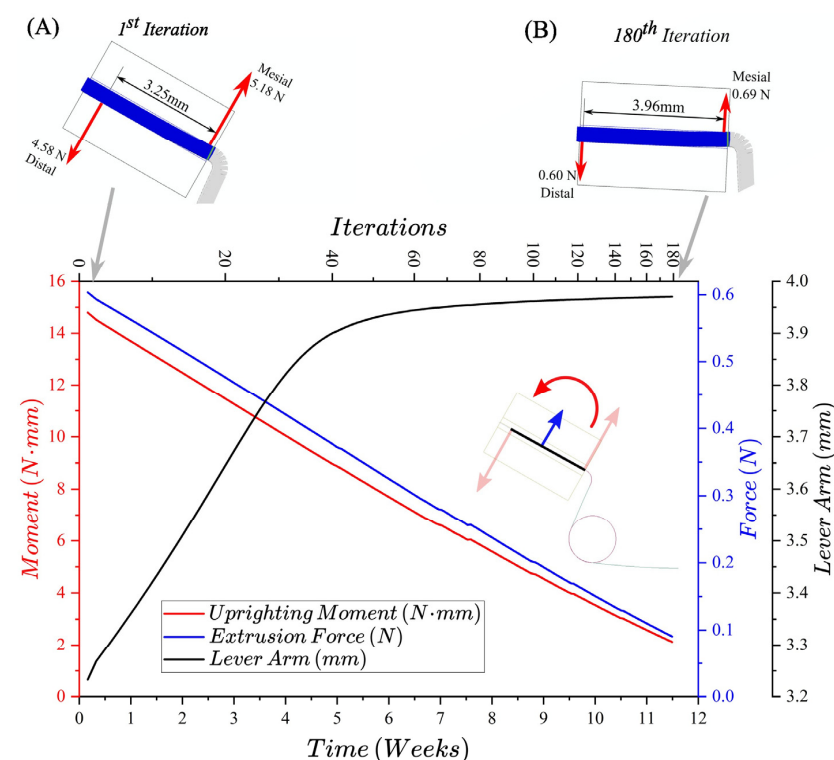


Figure 13. Force system acting on the mandibular second molar's buccal tube slot during the uprighting simulation. The uprighting moment (red), extrusion force (blue), and short lever arm length (black) are plotted over clinical time (bottom x-axis) and corresponding simulation iterations (top x-axis). The mesial and distal contact forces and the effective lever arm length are shown in the insets above the graph: (A) at the beginning of treatment; (B) at end of the treatment. The progressive decrease in load magnitudes and the corresponding increase in lever arm length as the force system changes is illustrated.

Table 2 shows the summarized biomechanical effects of the conventional molar uprighting spring, reported at 2-week clinical intervals. This table provides an overview of forces produced by the spring, the amount of tooth correction achieved, and the movement rate during orthodontic treatment, which can be considered a simplified clinical reference to support treatment planning without requiring prior knowledge of finite element analysis.

Table 2. Estimated clinical progression of mandibular second molar uprighting using a conventional uprighting spring based on FE simulation results.

Clinical Week	Molar Uprighting Angle (°)	Molar Vertical Extrusion (mm)	Uprighting Moment (N·mm)	Extrusion Force (N)	Second Premolar Intrusion (mm)
Week 0	0.32	0.04	14.6	0.6	0.002
Week 2	3.9	0.49	12.6	0.52	0.009
Week 4	8.06	0.94	9.98	0.42	0.133
Week 6	12.09	1.35	7.63	0.32	0.196
Week 8	15.89	1.68	5.6	0.24	0.262
Week 10	19.55	1.96	3.53	0.15	0.328
Week 12	21.9	2.13	2.12	0.09	0.374

4. Discussion

The findings of this study reject the null hypothesis as the iterative FE simulation yielded results that are consistent with published clinical outcomes in terms of uprighting angle, treatment duration, and biomechanical trends.

4.1. Correlation of Iteration Time with Real Clinical Time

By implementing previously outlined methodology (Figure 2) and integrating key parameters from previous literature, the present model was able to establish a correlation between the presented simulated findings and the actual clinical duration required for molar uprighting. A key component of this methodology's formation was the graph presented in Figure 3, which illustrates the relationship between applied force and canine displacement velocity. Such a relationship was established utilizing data compiled from multiple clinical studies [24,25]. The compiled data revealed that tooth movement velocities vary across studies under the same applied force. This variability arises due to differences in tooth anatomy, PDL properties, bone conditions, and experimental protocols. Despite these variations, the black curve represents an average trend rather than a single dataset and includes a broad range of clinical observations, making it a valuable reference for estimating orthodontic tooth movement under varying conditions. Model 1 simulation was conducted under retraction loads ranging from 10 to 800 cN, incorporating carefully selected material assumptions, property values, model interactions, and boundary conditions to ensure consistency with real clinical conditions. These considerations enhance confidence in the robustness of the current FE approach and its outputs. A key outcome of this process was the introduction of a novel technique that directly translates computational iterations into real clinical time, based on the PDL's biomechanical response and bone remodeling velocity (Figure 7).

Bone remodeling is driven by fundamental biological responses to mechanical loading, and these processes are not strictly limited to a specific tooth type [10]. For this reason, authors used data from canine retraction studies as an appropriate reference to aid in estimating treatment timelines in the present molar uprighting model.

One key advantage of using canine retraction data for time calibration is that they are derived from controlled clinical studies in which a constant orthodontic force is applied,

resulting in a relatively steady tooth movement velocity. This predictable behavior provides a reliable reference for interpreting displacement in study's simulation. In the FE model, the normal displacement at the PDL–root interface—driven by tooth movement—is transmitted to the PDL–bone interface, as the ligament naturally attempts to restore its original uniform thickness. Importantly, this normal displacement is directly proportional to the local mean stress in the ligament, which serves as the primary mechanical stimulus for bone remodeling. By correlating this stress-driven displacement with the known velocity of canine movement, bone remodeling rates can be estimated and iteration count can be converted into a biologically meaningful clinical timeframe. Thus, this approach offers a simplified, consistent, and physiologically grounded method for time-mapping in orthodontic simulations.

In the present study, the estimated treatment duration for achieving a 22° molar uprighting was equivalent to almost 12 weeks of real clinical time. This lies in agreement with clinical studies, as molar uprighting treatment duration can vary between 2 and 5 months, depending on the severity of tilted molar angle and the appliance used for treatment [1,31,32]. An *in vivo* study assessed two different molar uprighting utilities using CBCT images. Molar uprighting was achieved throughout a treatment period of 4 months. These results can be possibly attributed to using less forces for molar uprighting, thereby requiring more treatment time [33]. Another biomechanical study conducted a clinical comparison of different molar uprighting techniques. They found that using a conventional molar uprighting spring achieved an 18° molar inclination correction within 9 weeks, while miniscrew-assisted molar uprighting achieved a faster correction of 17° within 7 weeks [32]. In general, the average duration for molar uprighting treatment was estimated to be between 2 and 3 months, with a mean of 24.5° of improvement in titled molar angulation [31]. This validates the reliability of this study's FE modeling technique in demonstrating clinically representative results.

The process of clinical validation was based on conducting comparisons of current model-predicted outcomes with values reported in published clinical studies using conventional uprighting springs. The outcomes were treatment duration and the angular correction of the molar. Such comparisons focused on assessing whether the model's predictions fall within clinically observed ranges.

The clinical studies utilized were selected based on the use of conventional molar uprighting springs, the availability of quantitative treatment outcomes (e.g., degree of uprighting and treatment duration), and clearly defined treatment protocols. Preference was given to studies that used CBCT or radiographic follow-up and reported angular changes pertaining to mandibular second molar.

The present model predicted a ~22° uprighting completed over ~12 weeks. These values closely align with reported clinical outcomes: Musilli et al. (2010) observed an 18° uprighting in 9 weeks [32]; Martires et al. (2018) reported correction over 4 months [33]; and Roig-Vanaclocha et al. (2021) described an average improvement of 24.5° over 2–5 months [31]. This agreement supports the clinical relevance of current simulation results.

The model's ability to predict treatment duration can support orthodontic clinical monitoring. As the model has shown the expected duration for uprighting a certain degree of molar tilt, it would worth conducting a progress assessment with new orthodontic records once the targeted duration has been exceeded. Additionally, future studies analyzing different severities of molar tilt, may propose an estimated duration of uprighting in each category, which can serve as guides for efficient clinical measures. This will aid in proper treatment planning in complex cases, as presenting a general treatment timeframe to patients aids in their decision-making process.

4.2. Tooth Movement Produced and Clinical Implications

The biomechanics behind molar uprighting are often coupled with unwanted effects, including molar extrusion or uncontrolled tipping when using different molar uprighting methods [32,33]. Thus, a detailed analysis is necessary to better control the clinical outcomes of molar uprighting.

The present study evaluated the efficiency of a conventional molar uprighting spring in achieving the desired correction for a tilted molar. The presented results indicate that the molar experienced some distalization during the uprighting process, which may be attributed to the distal location of the C_{Rot}, influenced by the molar’s angulation and the line of action of applied forces [34]. Additionally, the vertical extrusion of the molar also occurred due to the uprighting spring’s short lever arm producing a higher force component on the mesial upper corner of the buccal tube slot, which is an expected outcome when using this type of appliance [6]. However, the 2.15 mm of molar extrusion observed is considered clinically significant, as each millimeter of posterior extrusion is estimated to open the bite anteriorly by 1.5–2.5 mm [35]. Therefore, the use of such uprighting springs might not be recommended for cases requiring the strict control of vertical dimensions. The achieved partial molar uprighting of about ~22° suggests that the further activation of the spring may be needed in order to achieve full molar uprighting. Furthermore, adding a vertical control component to this activation, such as an intrusion bend, could help mitigate the molar extrusion [7].

The anchoring teeth showed varying amounts of vertical intrusion, with the highest intrusion located on the second premolar, which can be attributed to the spring’s point of engagement with the anchorage wire being between the two premolars. This tilting in the occlusal plane indicates that, although the square 0.016-inch stainless steel consolidating wire is considered theoretically rigid, it still undergoes slight bending, therefore affecting the vertical position of the anchoring segment even when they are tied together. Incorporating a larger dimension consolidating wire or possibly adding a bonded retainer can reduce this unwanted effect on the anchorage teeth [13,36].

Although limited, the literature includes quantitative FE analysis and clinical data related to molar uprighting [13,15,31,32,37]. Table 3 illustrates a comparative overview of prior findings in relation to the current study’s outcomes. It also highlights the proximity of the achieved simulation results to common clinical observation.

Table 3. Current study’s simulation outcomes compared to previous FE analysis (FEA) and clinical data. Corresponding values that were not reported in some of the listed studies; these are marked with (-).

Author	Study Type	Molar Angular Correction (°)	Forces Used	Treatment Duration
Present Study	FEA	21.9°	0.6 N (~61 g)	12 Weeks
Kojima et al., 2007 [13]	FEA	22°	0.66 N	-
Zheng et al., 2024 [15]	FEA	-	0.5 N	-
Roig-Vanaclocha et al., 2021 [31]	Clinical Case Series	24.5° (Mean)	-	10–12 Weeks
Musilli et al., 2010 [32]	Clinical Study	18°	-	9 Weeks (9.1 Weeks) *
Bae and Kim, 2022 [37]	Case Report	-	50 g	12 Weeks

* The duration extracted from current model corresponding to an 18° molar angular correction.

While the assumptions of the current model were designed to be standard and reproducible, they closely resemble routine clinical practice. Sectional mechanics are highly predictable in comparison with a continuous archwire system [6]. They aid in creating

a controlled environment where variables can be set and assessed individually [7]. The present archwire setup and the second molar tilt of 30° with a missing first molar were chosen to mimic the nature of cases usually encountered in daily practice. Furthermore, this angular assumption was chosen based on a previous molar uprighting FE study [13] to aid in the comparative assessment.

The use of 2D FE modeling has been proven as a valid approach in the orthodontic literature. Subjects such as tooth movement simulation under specific force systems, inflected stress assessment, and distribution in the periodontal ligament and alveolar bone were previously investigated using 2D FE models [38,39]. In the current study, 2D modeling was used in order to simplify the simulation of long-term orthodontic tooth movement during molar uprighting, while maintaining accuracy to capture key biomechanical responses and provide reliable results for the iterative process. The rationale behind this was twofold. Firstly, we aimed to explore the sagittal-plane biomechanics of molar uprighting in an efficient and focused way. And secondly, we aimed to test the effectiveness of an iterative simulation process that updates tooth and PDL geometry over time while correlating simulation steps with real clinical treatment duration.

Utilizing a 2D FE model represents a scientifically justified simplification and is particularly suited for analyzing movements that predominantly occur in a single anatomical plane, where 3D effects such as torque and rotation are minimal. Romeo and Burstone (1977) quantified the moment required for molar uprighting using a conventional uprighting spring as being within the range of 12–17 N·mm, a value consistent with present study data [40]. Moreover, Romeed et al. (2006) showed that the distribution of maximum principal stresses in both alveolar bone and the PDL was comparable between 2D models and the corresponding sagittal sections of 3D models, supporting the relevance of 2D analysis under planar movement conditions [41]. Complementarily, the 3D FE study by Kojima et al. (2007), which employed the same type of uprighting spring as in current study, demonstrated that when the spring arm is not pre-bent, the uprighting of a molar by 22° is associated with a bucco-lingual tipping angle of less than 1° [13]. This confirms that the displacement remains mainly within a two-dimensional configuration, thus supporting the relevance of a 2D modeling approach for the specific objective of simulating molar uprighting mechanics. This approach allowed for establishing a new framework for long-term orthodontic simulation, which could lay the groundwork for more complex 3D modeling in future studies.

4.3. Contact Forces and Load Transfer Mechanics

Supporting oral tissues can withstand orthodontic forces up to a biological threshold, beyond which excessive uncontrolled forces lead to undesirable effects [42]. In the current simulation, the extrusion force generated on the molar was around 0.6 N (61 g), which lies within the range of optimum forces for orthodontic tooth movement [43]. Some studies suggested that forces up to 150 g are considered to be biologically acceptable for molar uprighting [44]. In general, molar uprighting forces should not be more than 1 N [45], and the moment produced should not exceed 1500 g·mm [46], which is in agreement with the present results.

Another interesting finding throughout the molar uprighting simulation was the 0.71 mm progressive increase in the spring's short lever arm length over the course of treatment, which occurred without any wire sliding. This phenomenon can be explained by the spring's relaxation, force decay, and evolving contact force distribution during the uprighting process. We were able to analyze this change by considering the interplay between the molar buccal tube slot and the uprighting spring wire, a factor overlooked in previous studies [13,16].

At the beginning of the treatment simulation, the spring wire was highly deflected due to the initial bending moment generated by the prescribed rotation applied to the arm of the uprighting spring in order to anchor it to the anchorage wire. Due to the tilted inclination of the molar, the mesial contact was relatively concentrated at the upper corner, while the distal contact was more distributed along the lower inner wall of the buccal tube slot. The resultant distal force acted farther from the distal edge, reducing the effective lever arm length to approximately 3.25 mm, which was notably shorter than the full slot width of 4 mm. This resulted in an unbalanced force distribution with a larger mesial–upward contact force and a smaller distal–downward force, producing both a counterclockwise moment and an extrusion force on the molar.

As uprighting progressed and the deformation of the wire diminished, the spring no longer remained curved but instead adopted a more oblique alignment within the buccal tube slot, making contact primarily at the upper mesial and lower distal corners. This shift allowed the mesial and distal contact forces to migrate toward the outermost edges of the 4 mm wide slot, increasing the effective lever arm length to approximately 3.96 mm by the end of the treatment. With this realignment, the spring transmitted lower and more symmetrically distributed forces to the molar, generating a substantially reduced counterclockwise moment and extrusion force by the end of the treatment simulation. These findings underscore the importance of accounting for evolving force contact points within brackets and buccal tubes during treatment, as they can significantly influence the applied force system, the resulting tooth movement, and ultimately, orthodontic treatment outcomes [36].

The current 2D simulation possesses a challenge in real orthodontic clinical setup scenarios. As the second-order dimension is thoroughly assessed, the remaining first-order and third-order movements cannot be visualized. However, given the couple force system generated at the molar tube, the resulting second-order correction, including the mesio-distal molar tilt, should be, in general terms, independent of changes in other dimensions [13,36]. Nevertheless, the current data must be interpreted with this 2D limitation in mind, until further analysis with 3D comprehensive modeling is carried out in the future.

4.4. Bone Remodeling and Average Mean Stress in PDL

PDL stress is considered a key trigger for the bone remodeling process and plays a crucial role in regulating orthodontic tooth movement [10,47]. The present study's FE model demonstrated a consistent relationship between PDL's normal displacement and average mean stress throughout the molar uprighting process, which aligns with previous findings that suggest a linear correlation between tooth movement rate and PDL stress [48]. The optimal PDL stress range that promotes tooth movement has been reported to be between 0.47 KPa and 16 KPa [47]. This is reflected in the presented findings, where the highest bone remodeling velocity observed was for an average mean stress in PDL ranged between 14 and 18 KPa. Overall, the highest PDL stress value produced by the conventional molar uprighting springs was around 28 KPa, which still remains within the acceptable range, as previous studies have suggested that even stresses up to 39 KPa were suitable for some orthodontic tooth movements, such as canine distalization [49].

The consistent ratio observed between the PDL's normal displacement and mean stress during molar uprighting indicates that for every 1 KPa of mean stress, the PDL undergoes a normal displacement of approximately 0.41 μm . This observation is in agreement with the tooth displacement and bone remodeling rates predicted by current finite element models, which yielded an average stress-normalized bone remodeling velocity of $\sim 0.9 \mu\text{m}/(\text{KPa}\cdot\text{day})$, closely matching the values reported in the literature [50].

Previous molar uprighting simulations treated the alveolar bone as a rigid structure [13]. In contrast, to better reflect clinical conditions, we modeled the alveolar bone as an elastic material, since material properties significantly influence FE outcomes, particularly the behavior of the PDL, which plays a critical role in determining the bone remodeling velocity [21,51,52].

The PDL was modeled as a linear elastic material to balance computational efficiency with biomechanical relevance. Although the PDL exhibits nonlinear and viscoelastic properties, linear elasticity is widely used in FE studies as it captures the overall stress distribution trends needed to trigger long-term tooth movement, particularly in iterative analyses. The linear assumption is further supported, as the PDL's stress–strain behavior is approximately linear under moderate orthodontic loading conditions, similar to the characteristics of conventional uprighting springs.

4.5. Future Work

For future consideration, expanding the current analysis to a 3D-model simulation would offer a more comprehensive understanding of the biomechanical effect of conventional molar uprighting spring on the involved oral structures, particularly in the buccal-lingual direction. Furthermore, including a targeted sensitivity analysis, such as using varying material properties, PDL geometry, and spring activation angles, to evaluate how variations in input parameters may influence displacement patterns, load transfer mechanism, and treatment duration predictions, would strengthen the robustness of conclusions and offer insights into model stability. Additionally, such investigation may assist in revising current clinical practice, including decisions, the re-activation frequencies of the uprighting springs during follow-up appointments, or possibly adding additional components to improve force control and tooth correction. Common orthodontic procedures, such as wire cinching and its impact on the force system, could also be investigated. Furthermore, creating future FE models that analyze alternative appliances, such as miniscrew-supported uprighting springs, could provide important findings that further enhance the understanding of molar uprighting biomechanics. In this study, the number of iterations in the FE model was successfully translated into real clinical time, making this, to the authors' knowledge, the first study of its kind. This advancement provides a new perspective for future FE investigations and opens the door for the potential prediction of both treatment progression and duration when using various orthodontic appliances. It also paves the way for more detailed 3D CAD modeling to assess how much out-of-plane effects influence the overall biomechanics and the validity of the notion of 2D simplification.

5. Conclusions

Understanding the biomechanics behind molar uprighting springs is essential for enhancing clinical treatment outcomes. The FE model in the present study illustrated the biomechanical effects of a conventional molar uprighting spring. This spring exerted forces that produced molar uprighting of around 22° , with 2.15 mm of vertical extrusion, in a span of 12 weeks in clinical time. The average stress-normalized bone remodeling rate was around $0.9 \mu\text{m}/(\text{KPa}\cdot\text{day})$, and the highest rate of tooth movement occurred between week 4 and week 6 of treatment. These findings can be used as a base for future comparison with different molar uprighting appliances. This study has shown the potential use of a novel FE modeling technique as a method for estimating the clinical treatment duration required for orthodontic tooth movement. This creates an opportunity for new horizons in orthodontic FE research, with the ultimate goal of improving clinical efficiency and optimizing the overall treatment provided to patients.

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