

Article

Biomechanical Effects of Different Auxiliary–Aligner Designs on the Rotation of an Upper Canine: A Finite Element Analysis of a Specific Patient

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Abstract: Aim: The objective of this research has been to apply a specific simulation to a patient to assess the biomechanical consequences of rotating an upper canine tooth through different attachment–aligner configurations and to predict the most efficient design using a three-dimensional finite element model of a full maxillary arch of a specific patient. Materials and methods: This was obtained by combining Cone-Beam Computed Tomography (CBCT) with the aim of reconstructing tooth roots and bone tissues, and Surface Structured-Light Scanning for creating digital tooth crown models from the patient’s impressions. This model was imported into the finite element solver (Ansys® 17). Three different attachment–aligner combinations were created through the exploitation of computer-aided design (CAD) procedures, i.e., without attachments, with a couple of attachments and with an attachment and a pressure point. For each simulation, the resulting force–moment (MF) system applied by the aligner to the target tooth, as well as the tooth displacement and rotation, was computed using a workstation based on Intel Xeon CPU E3-1245 v3@3.40 GHz and 16 GB RAM. Simulations reported that by adding the pressure point and the attachment to the standard aligner the amount of Moment z (Mz) delivered to the tooth increased almost two times. Results and conclusions: The maximum tooth displacement (0.85 mm) was obtained with the attachment and pressure point aligner, while the lowest (0.058 mm) was obtained with use of a couple of attachments. Both the attachment and the pressure point have the potential to enhance the appliance’s effectiveness. Particularly, the pressure point showed a higher influence on the load absolute value. The method applied in the present study should be used to retrieve the best design configuration for each patient and specific tooth movement.

Keywords: finite element analysis; aligners; malocclusion; orthodontic movement; digital workflow; three-dimensional tooth movement; three-dimensional diagnosis and analysis



Citation: D’Antò, V.; Bocchino, T.; Levatè, C.; Buono, R.; Razionale, A.; Barone, S.; Savignano, R. Biomechanical Effects of Different Auxiliary–Aligner Designs on the Rotation of an Upper Canine: A Finite Element Analysis of a Specific Patient. *Appl. Sci.* **2024**, *14*, 2308. <https://doi.org/10.3390/app14062308>

Academic Editor: Jong-Moon Chae

Received: 22 November 2023

Revised: 27 February 2024

Accepted: 7 March 2024

Published: 9 March 2024



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1. Introduction

Achieving a high level of predictability in an orthodontic treatment has consistently proven to be a motivating and demanding challenge to orthodontists, primarily due to various factors that could influence the clinical outcome. That is why a better understanding of how to achieve tooth movements would allow the design of optimized appliances, leading to more efficient orthodontic treatments.

However, in addition to playing an important role in smile aesthetics and functional occlusion, the accurate positioning of the maxillary canines that support the alar base and upper lip should be the goal of orthodontic treatment [1].

Today, thanks to improvements in the biomechanics and physical characteristics of materials [2], aligner therapies have the possibility to treat several case typologies such as Class II, Class III and interdisciplinary cases [3–5] with an efficacy comparable to that of braces, differently from the early age where clear aligners were only considered to treat simple orthodontic problems like mild or moderate anterior crowding. The use of auxiliaries and attachments with aligners is widely adopted in clinical practice thanks to the good mechanical and chemical properties of the aligners [6,7], and to the advantages in using removable appliances which require fewer emergency visits and allow better oral hygiene, increasing the possibility to achieve complex movements such as rotation or torque [8].

The digital workflow to design and manufacture orthodontic aligners relies on the digital reconstruction of a patient's anatomy and CAD/CAM (computer-aided design/computer-aided manufacturing) techniques [9,10]. Specialized dental technicians use CAD systems to segment the digital patient's anatomy, creating separate objects for each tooth and soft tissues. Afterwards, following geometrical and functional constraints, the technicians reposition the teeth to develop a digital treatment plan: the entire treatment is then divided into smaller sequential tooth movements, from the baseline condition to the final expected outcome. For each treatment step, a 3D model of the dental arch is 3D-printed and the customized appliances are then produced from the 3D-printed models by a vacuum thermoforming process.

The current workflow is based mainly on the analysis of tooth crown positions, with little consideration for the root movements. This approach could lead to erroneous estimations of the location of the tooth's center of resistance and to dangerous interferences with roots during the treatment, compromising its outcome.

The rotation movement of conical-shaped teeth is considered a difficult movement to achieve with clear aligners. According to a prospective study realized on 53 maxillary canines, the mean accuracy of the rotation movement was 36% [11]. For this type of movement, the maxillary canine reports an accuracy lower than other teeth such as the maxillary central incisor (55%) and the mandibular central incisor (52%). The lowest accuracy was noticed for the mandibular canine, reporting an accuracy of 29%. The accuracy of the rotation movement was significantly reduced for rotations greater than 15° (19%) [12]. Additionally, another study investigating the mesiodistal angulation of canines with fixed orthodontic treatment revealed the importance of movement control of the lower canines, especially in orthodontic mechanics in the mandible, due to the increase in the mesiodistal angulation of the lower canines in all malocclusion groups [13].

In these studies, the accuracy of tooth movements, such as rotation or distalization, was calculated by superimpositions of virtual models by using reference surfaces such as palatal rugae, untreated teeth and dental implants [8,11,12]. By comparing pretreatment optical 3D scans with the virtual plan and with the post-treatment optical 3D scan, it was possible to calculate the accuracy of different tooth movements. Nevertheless, this technique has some limitations which involve manual landmark identification and the stability of the reference areas used for the superimposition.

Finite element analysis (FEA) is a computational technique that has been applied the most to understand the transfer of the force from the application point to the alveolar structures via the PDL, and FEA allows the calculation of biomechanical parameters such as force, pressure and thermal changes obtained on biomaterials and human tissues and that can be hardly measured *in vivo* [14].

Finite element simulation could lead to a prediction of the biomechanical effects of different orthodontic appliances; a previous study evaluated the effects of a rapid maxillary expansion on the craniofacial skeleton of a patient with unilateral cleft lip and palate to individuate the application of points of force for a better expansion using a three-dimensional finite element model [15].

With the aim of identifying the mechanics of the teeth whose movement is planned, as well as the effects on dental elements that act as anchorage, there have been few attempts to study tooth-aligner interactions by finite element models (FEM) [16–18]. Some studies have

investigated the effects deriving the M:F ratio from the presence and type of attachments when a translation movement is planned. Regardless of the attachment, movement occurs initially by tipping, while the pair of forces for root control and uprighting only occurs later if attachment is present; when there is no attachment, tipping is the only expected result [19]. Moreover, an overhanging attachment appears to be able to control unintentional tooth movement better than general attachment [20]. Another key point is the position of the attachment: during incisor extrusion, a rectangular palatal attachment could improve the biomechanics and therefore the effectiveness of the planned movement [21].

As we have seen, one of the main features of orthodontic aligners that characterize the force transfer from the aligner to the tooth is the auxiliary elements, like attachments, divots and power ridges. Their geometrical features and positions strongly affect the load transfer and therefore the tooth movement [22]. For this reason, it would be desirable to optimize their features using numerical methodologies, such as the finite element method (FEM).

Numerical methodologies would allow orthodontic behaviors to be simulated. In recent years, research activities have been focused on the analysis of traditional orthodontics, contrary to what was carried out for the biomechanical modelling of aligner treatments [23]. A patient-specific 3D finite element model (FEM) was developed to analyze the biomechanical response using different auxiliary elements to correct malocclusion. The patient anatomy was digitally reconstructed by merging optical 3D scanning and Cone-Beam Computed Tomography (CBCT), thus providing an accurate model comprising tooth crowns, roots periodontal ligaments (PDLs) and alveolar bone. The orthodontic appliance was modelled by exploiting Boolean operation through AutoCAD® (Autodesk®, Q.104.0.0 AutoCAD 2020.1.2, <https://www.autodesk.com/>) to replicate the appliance manufacturing process. FEA simulated the interactions between anatomical tissues and appliance structures, enabling both the geometrical and mechanical attributes of the appliance to be tuned to gain the target tooth movements.

In the current literature, there is not any example of a specific clinical case treated with an aligner configuration chosen according to an FEA simulation: the aim of the current paper was to simulate the rotation movement of a maxillary canine for a specific clinical case by using three different aligner configurations, and to predict with a fully digital workflow the most efficient aligner design and auxiliaries.

2. Materials and Methods

The present study displays an innovative method for the aligner treatment planning based on the tissue response to the orthodontic loading during the initial stages for a specific patient.

The presented method describes an integration of numerical analysis into clinical treatment planning. The anatomical structures are reconstructed by merging Cone-Beam Computed Tomography (CBCT) and optical 3D scanning datasets. Afterwards, finite element analysis (FEA) is conducted for different aligner–auxiliary combinations. The numerical results (tooth displacement and force system delivered by the aligner) lead to the selection of the most effective aligner treatment plan. The application of this method to the treatment of a case is described step by step (Figure 1).

2.1. Clinical Case

M.S. is a female 17-year-old patient who sought treatment at the Department of Orthodontics at the University of Naples “Federico II”, and in the end she gave consent to the publication of the records and the results obtained.

She presented an oval face and a good smile exposure with a 1 mm right deviation of the upper middle line with respect to the facial middle line. She has an orthognathic and retrusive profile, and increased chin–neck distance and flattened cheekbone contouring. At the intraoral analysis, there was persistence of the deciduous maxillary right canine and the absence of the corresponding permanent tooth. She had both molar and canine class I relationship on both sides, minimal crowding (1 mm), a 2 mm overjet (OVJ) and a 2 mm

overbite (OVB). White spot lesions (WSL) due to a previous orthodontic treatment were present on most of the dental surfaces. She was in permanent dentition and at panoramic X-ray analysis we could see the inclusion of the maxillary right permanent canine (Figure 2).

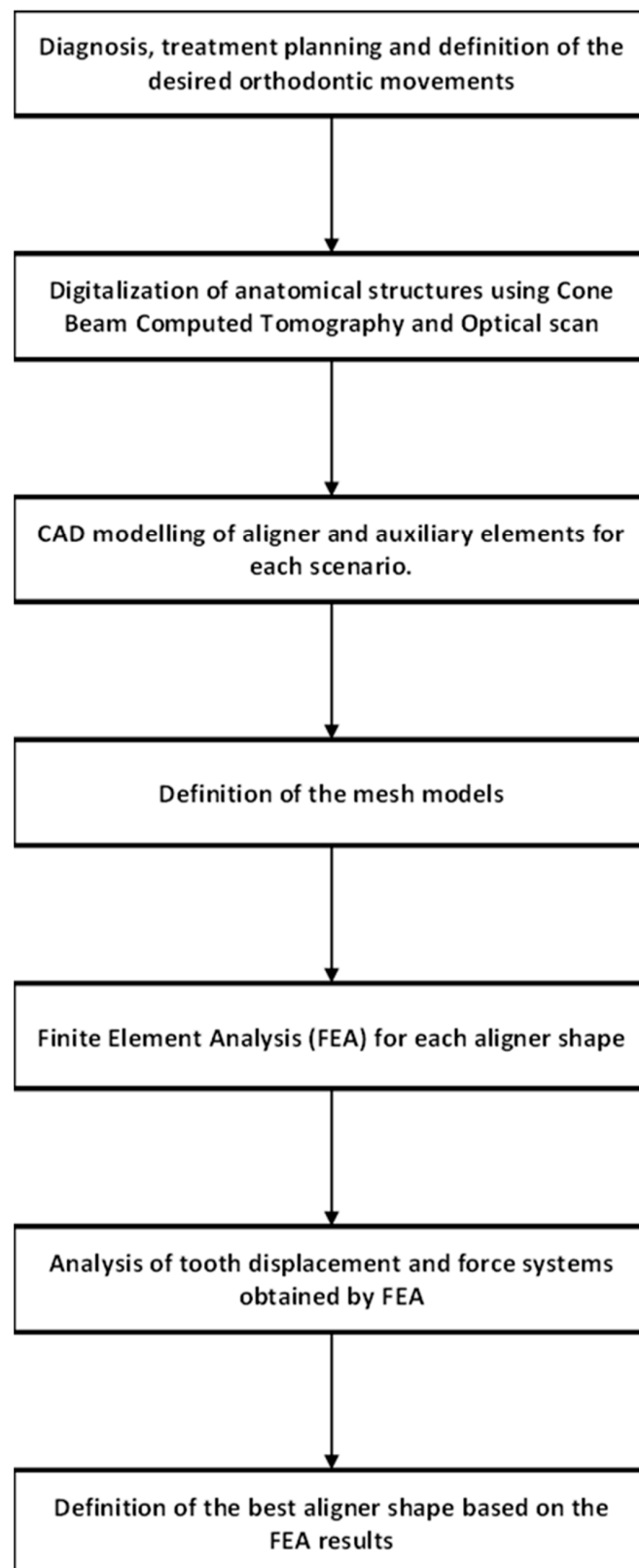


Figure 1. Flowchart of the proposed model.

A skeletal III class with a bi-retrusion and a brachi-facial growth pattern resulted from the cephalometric EBO analysis results (Table 1).

In this patient, the treatment plan needed to provide the recovery of the impacted canine: the first step was surgical exposure of the canine crown, then the canine was pulled through a Temporary Anchorage Device (TAD) [24,25]. At first, the canine was surgically exposed then, a miniscrew OrthoEasy® (FORESTADENT Bernhard Förster GmbH, Pforzheim, Germany) 10×1.7 mm was inserted from the palatal side between 1.5 and 1.6, and a Titanium Molybdenum Alloy (TMA) rectangular wire (0.019×0.025) was used to shape a lever activated to pull the palatal canine (Figure 3).

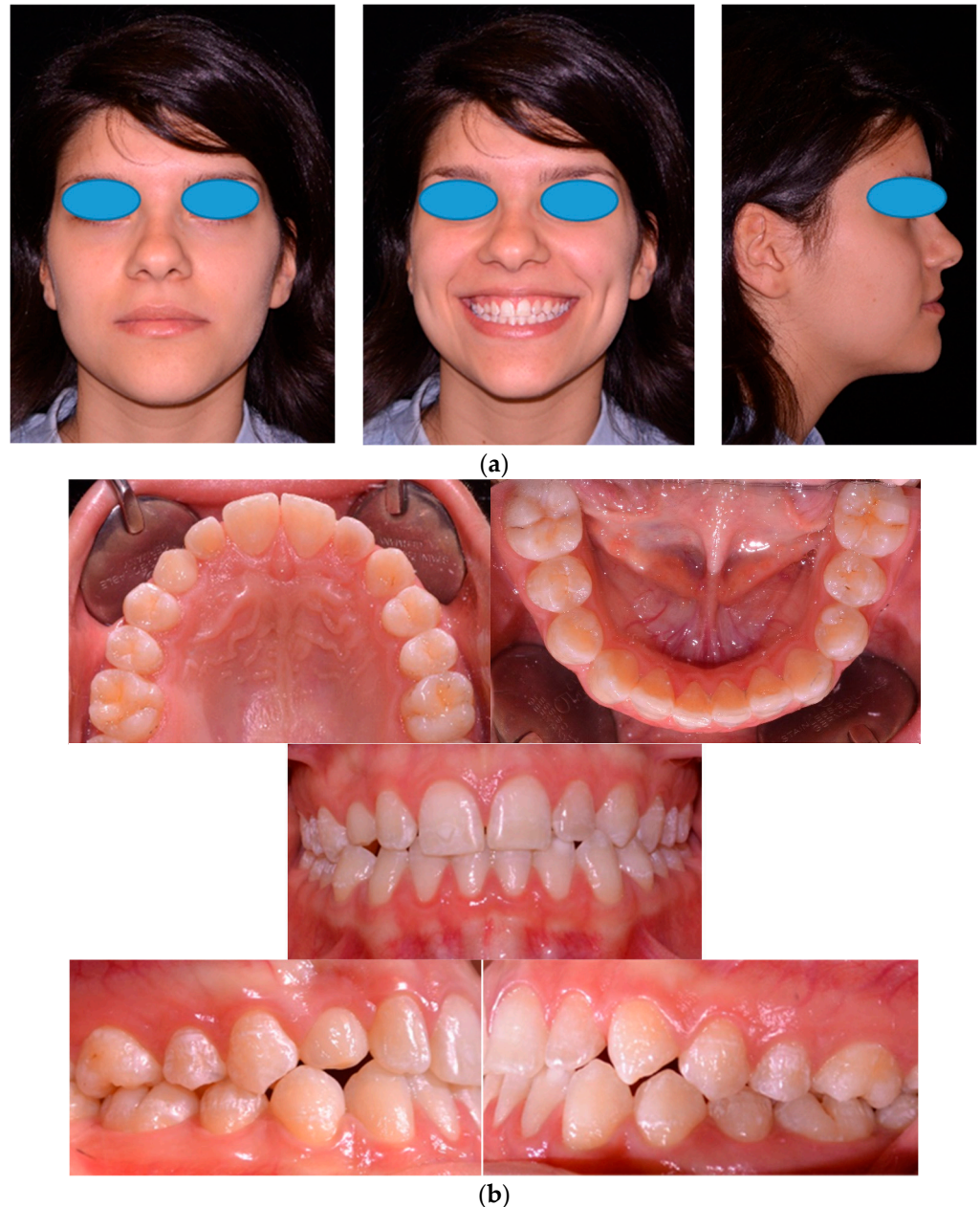


Figure 2. Cont.

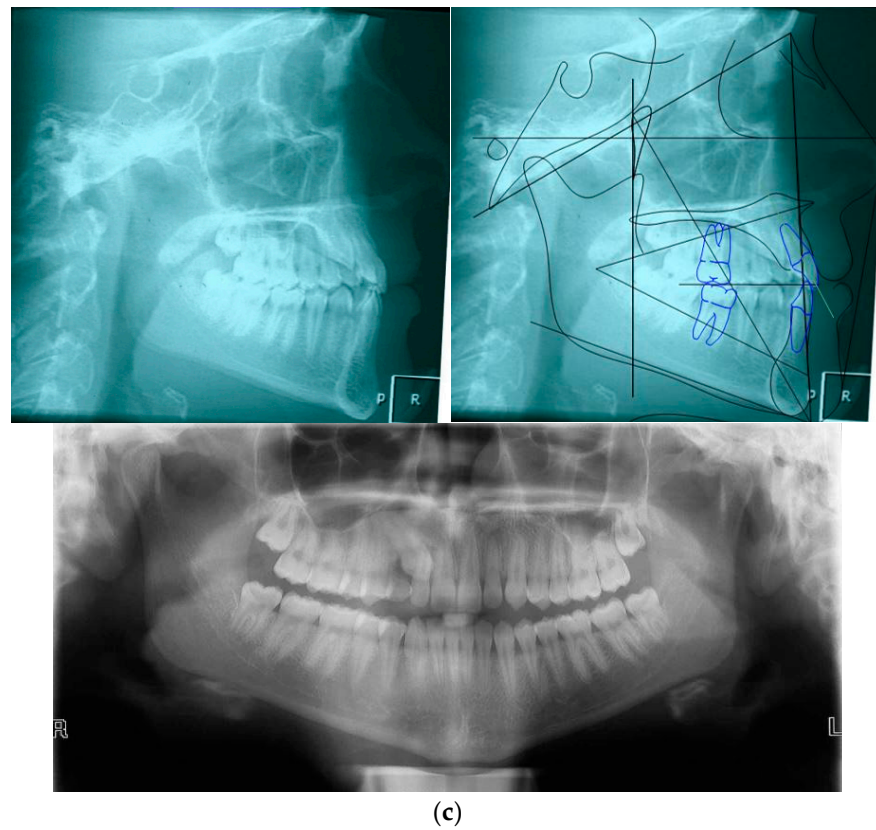


Figure 2. Initial documentation: extra-oral (a) and intraoral photographs (b), cephalometric tracing, teleradiography and panoramic X-ray (c).

Table 1. Cephalometric data before treatment.

Sagittal Jaw Relationship		
	Patient Value	Normal Value
Maxillary position SNA (°)	81.4	82 ± 3.5
Mandibular position SNB (°)	81.8	80 ± 2.5
Sagittal jaw relation ANPg (°)	−0.4	2 ± 2.5
Vertical jaw relationship		
Maxillary inclination SN^ANS-PNS (°)	5.7	8 ± 3
Mandibular inclination SN^GoGn (°)	28.4	33 ± 2.5
Vertical jaw relation ANS/PNS^GoGn (°)	25.5	25 ± 6
Dento-basal relationship		
Maxillary incisor inclination U1^ANS-PNS (°)	111.9	110 ± 6
Mandibular incisor inclination L1^GoGn (°)	81.8	94 ± 7
Mandibular incisor compensation (L1-Apo) (mm)	1.5	2 ± 2
Dental relationship		
Overjet (mm)	2.9	3.5 ± 2.5
Overbite (mm)	2.1	2.5 ± 2.5
Interincisal angle (°)	143.5	132 ± 6

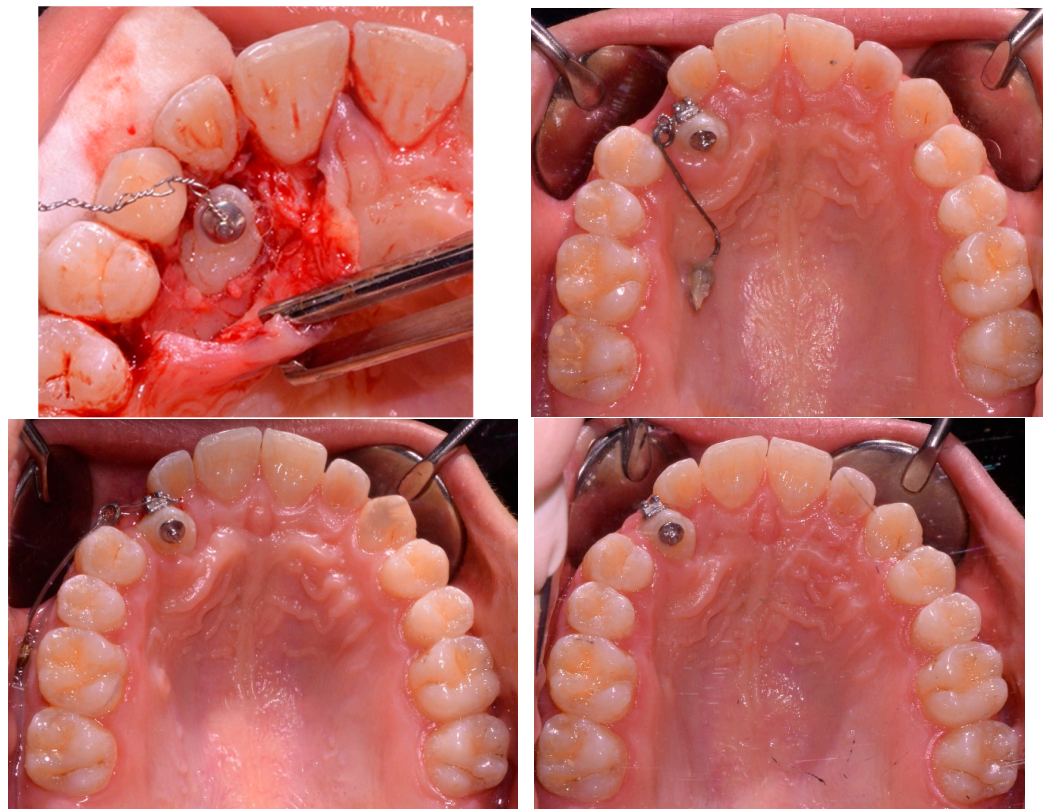


Figure 3. Canine recovery.

After the disinclusion, the canine was correctly positioned, and this could be achieved by a traditional fixed orthodontic treatment (brackets) or by aligners.

According to the literature, we classified this patient in the “high-risk” group for the onset of WSL [26], so we decided to treat her with a set of aligners. Moderate-quality evidence reveals less plaque accumulation and less salivary caries-associated bacteria in clear aligners, which might be related to the reduced incidence and severity of WSLs associated with CA when compared with fixed-multibracket appliances [27].

When the tooth was close to its correct position, the patient was ready to start the treatment with aligners. Figure 4 shows the patient’s documentation before starting treatment with aligners.

2.2. Finite Element Analysis

2.2.1. Reconstruction of the Patient’s Anatomical Tissues

The patient’s anatomical model was digitalized by combining two different imaging techniques: CBCT and intraoral 3D scan. The intraoral 3D scan of a plaster model created from the patient’s impression was used to create a digital model composed of tooth crowns and oral soft tissues. The resulting digital object was then segmented to separate the individual crown geometries and the gingiva.

The CBCT data, stored in a sequence of Digital Imaging and Communications in Medicine (DICOM) images (slices), were used to reconstruct tooth roots and bone tissues. The alveolar bone was segmented by processing the same CBCT data. For each slice, the regions outlined by the detected tooth contours were subtracted from the area obtained by the optical 3D scanning and were merged with the data from the CBCT, resulting in the most accurate representation for each tissue: i.e., tooth crowns by optical 3D scanning and tooth roots by CBCT imaging.



Figure 4. Documentation before starting aligner treatment: extraoral (a) and intraoral photographs (b).

The PDLs are not discernible with a CBCT exam, due to their minimal thickness (0.1–0.2 mm) [28]. For this reason, the PDLs were manually created by adding a 0.2mm shell to the area at the intersection between the bone and tooth models. The shell volume was then subtracted from the alveolar bone to obtain the PDL volume [29].

The aligner was designed with a uniform 0.7 mm thick object, which originates from the mean thickness of the thermoplastic material disk (0.75 mm thick) before the thermoforming process [30].

2.2.2. Definition of FEM Model

According to Savignano and co-authors, the reconstructed digital models were imported within the finite element modeler (Ansys® 17, Canonsburg, PA, USA). All bodies were meshed by using solid elements. In this study, a full maxillary arch composed of 14 teeth was modelled (Figure 5) [21].

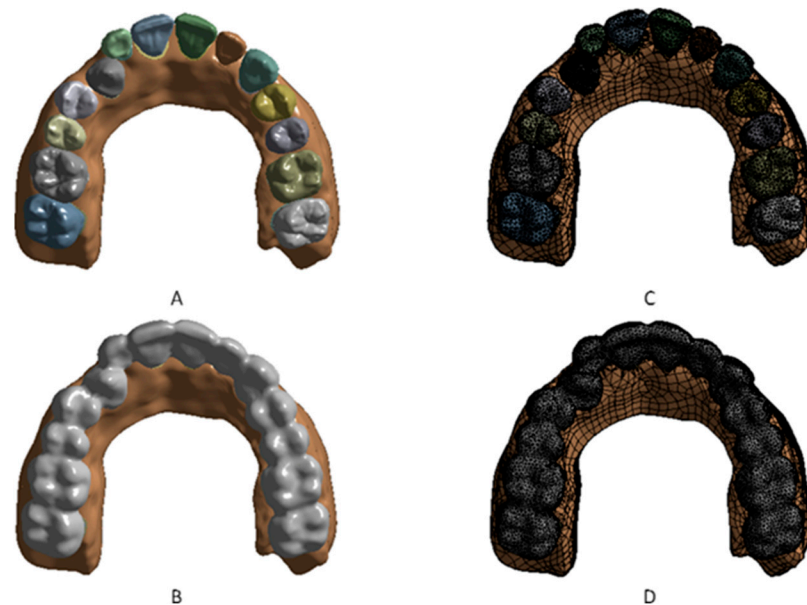


Figure 5. Geometrical models of the patient's anatomy without (A) and with the aligner (B). Finite element models of the patient's anatomy without (C) and with the aligner (D).

The load is transferred through the aligner–tooth contact surface and the initial penetration between the bodies defines the load features. Therefore, the mesh quality on tooth crowns and aligner inner surface must be high to preserve the ideal desired penetration within a certain tolerance range.

2.2.3. Mechanical Properties

According to Barone and co-authors, all bodies were modelled as linear elastic and teeth and bone were assumed to be made of a homogenous material, without discerning between substructures [23]. This simplification does not influence the simulation results as demonstrated in previous studies [28,31–33]. In the technical literature, there are many biomechanical models that simulate the tooth ligaments' properties [9]. Depending on the focus of the simulation, different models can be used. They can be categorized into five groups: linear elastic, bilinear elastic, viscoelastic, hyperelastic and multiphase [34]. A linear elastic model is justified for the present study, which focused on the first phase of the orthodontic reaction [31]. The removable appliances have been simulated as made of a polyethylene terephthalate glycol-modified (PETG) thermoplastic disc. Attachments have been assumed to be made of the same tooth material.

2.2.4. Boundary Conditions

The bone extremity nodes were not allowed to move in any directions. Bonded contacts were defined between the bone and PDLs and viceversa, simulating perfect adherence between contact surfaces, without mutual sliding or separation [23].

The contact surface between the aligner and teeth was modelled by using a frictionless model, allowing load transfer between the two bodies and mutual movements. Neglecting friction is a reasonable choice due to the presence of saliva and to the differences between the thermoplastic material of the aligner and the enamel [23].

The non-linear simulation was solved by using the Newton–Raphson residuals method based on the force and moment convergence values. The number of initial sub steps for each simulation was set as 100 while the contact stiffness was automatically updated at each iteration.

The maximum contact penetration allowed at the end of the simulation was defined as 0.01 mm. The minimum initial penetration among the three simulated configurations was 0.117 mm (Figure 6); therefore, a tolerance value of 0.01 mm was lower than the 10% of the initial geometrical mismatch. This value was determined by considering that higher values significantly affect the results while lower values increase convergence time without entailing significant changes in the results.

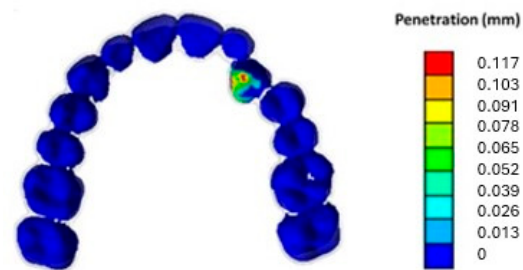


Figure 6. Initial penetration between teeth and aligner. The value is null for all the teeth except for the maxillary canine, which has to be moved by the device.

2.2.5. Analysis Settings

We carried out simulations to evaluate the aligner's effectiveness in three different configurations: aligner without any attachment, aligner with a couple of attachments and aligner with an attachment and a pressure point (Figure 7).

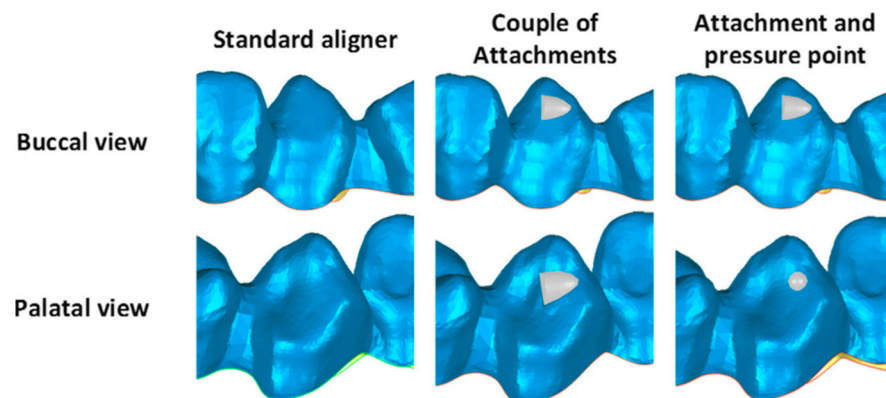


Figure 7. Buccal and palatal views of the different aligner shapes analyzed during the present study. Auxiliary elements are highlighted in white.

For each simulation, the resulting force–moment (MF) system delivered by the aligner to the tooth and the tooth movement and rotation were calculated. The MF was calculated at the tooth's center of resistance (Cres). The computational time resulted to be about 6 h for each simulation, using a Workstation based on Intel Xeon CPU E3-1245 v3@3.40 GHz and 16 GB RAM [18].

Figure 8 shows the intraoral photographs with the first couple of aligners.



Figure 8. Intraoral photographs at the beginning of the aligner treatment.

3. Results

The FEA results were analyzed for each configuration by comparing the moment along the z-axis and the resulting moment-to-force-ratio (M:F) delivered to the tooth on the XY plane. The M:F values describe the quality of the force system [35], while the absolute values of M and F define the amount of orthodontic movement. Figure 9 reports the displacement occurring for each simulation.

Table 2 shows how the combination of pressure point and attachment produced the maximum tooth displacement (0.085 mm), which is justified by the higher forces and moments measured at the tooth CRES compared with the other configurations.

Table 2 also shows high force and moment values for the standard aligner; however, the loads are not in the desired directions, as demonstrated by Figure 8, in which one can notice that with the standard aligner the resulting movement is approximately a mesiodistal tipping of the maxillary canine.

Figure 10 shows the patient's documentation at the end of the orthodontic treatment carried out by using AirNivol (AirNivol S.p.A., 56023, Cascina, (PI), Italy) [36] aligners.

Table 3 shows the cephalometric data of the patient at the end of treatment.

The stability of the obtained results were analyzed after four years (Figure 11).

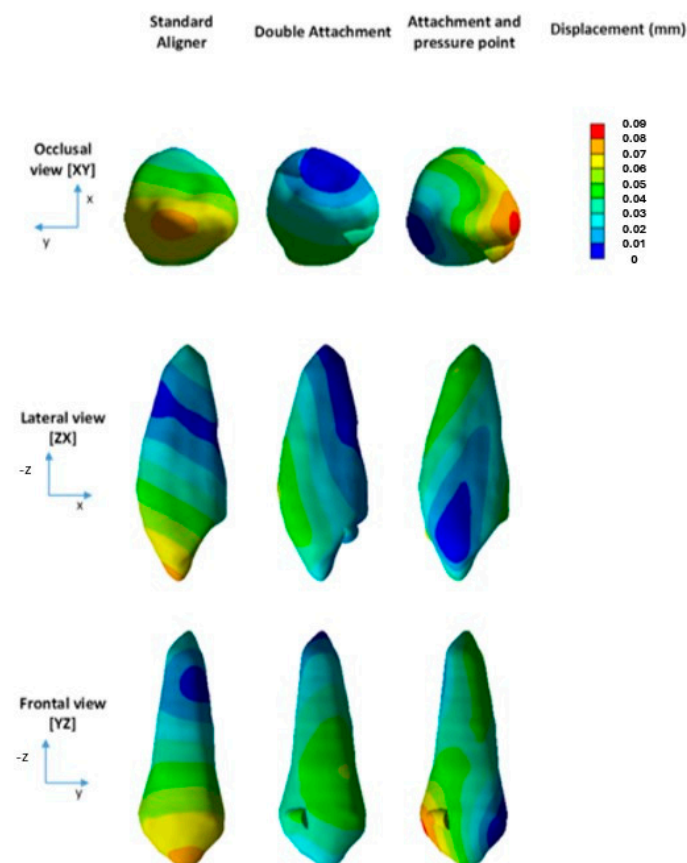


Figure 9. The displacement occurring for each simulation is shown by the different views. It can be seen how the activation point with attachment generated the maximum displacement (red). Moreover, the approximate center of rotation can be retrieved for each simulation as it is located in the blue region.

Table 2. Maximum displacement and loads delivered to the tooth by the different aligners. The force systems are measured at the tooth's center of resistance.

	Standard Aligner	Double Attachment	Attachment and Activation Point
Maximum displacement (mm)	0.075	0.058	0.085
Fx (N)	−0.36	−0.26	−0.64
Fy (N)	−0.93	−1.53	−3.62
Fz (N)	−1.5	−1.09	−3.75
Mx (Nmm)	4.23	0.79	−4.3
My (Nmm)	1.1	−1.23	11.5
Mz (Nmm)	7.6	5.77	12.3
Mz/Fx (mm)	−19.5	−22.2	−19.21
Mz/Fy (mm)	−8.2	−3.8	−3.4
My/Fx (mm)	6.7	4.73	−17.8
My/Fz (mm)	5	1.13	−3.1
Mx/Fy (mm)	−11.7	−0.51	1.2
Mx/Fz (mm)	−3.7	−0.72	1.2



(a)



(b)

Figure 10. Cont.

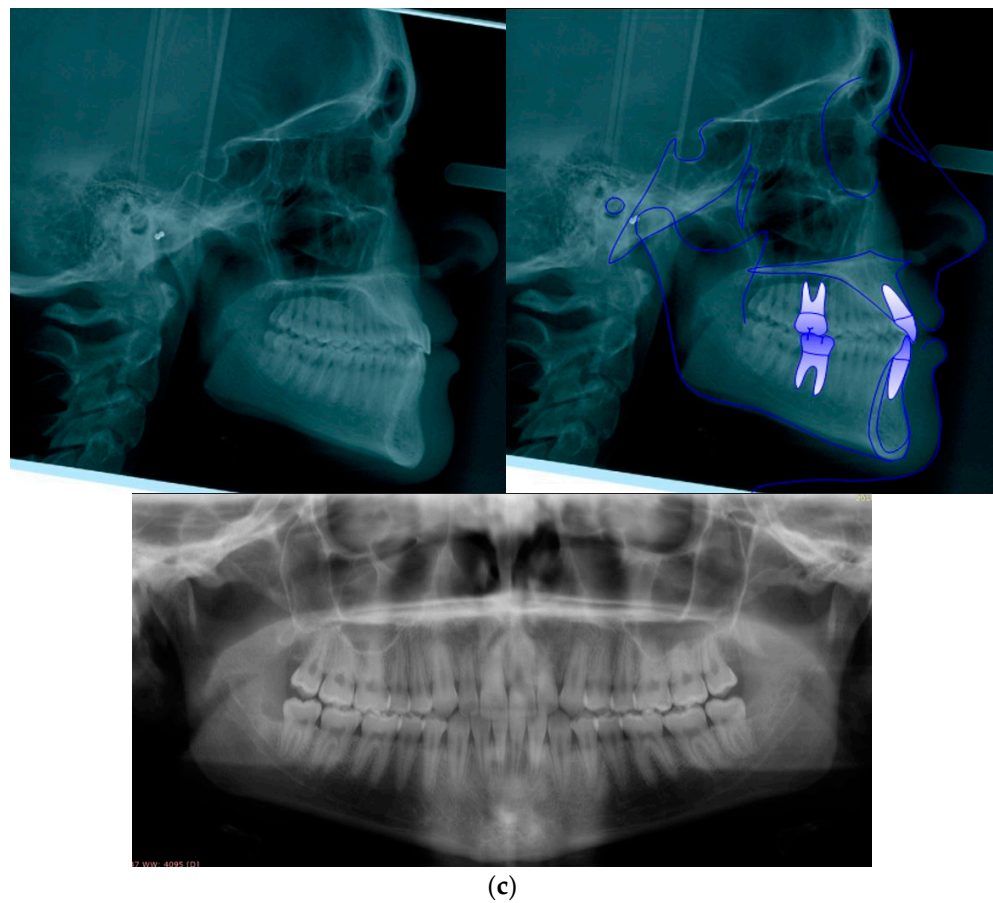


Figure 10. Patient's documentation at the end of the orthodontic treatment: extraoral (a) and intraoral (b) photographs and radiographic evaluation (c).

Table 3. Cephalometric data at the end of treatment.

Sagittal Jaw Relationship		
	Patient Value	Normal Value
Maxillary position SNA (°)	80.7	82 ± 3.5
Mandibular position SNB (°)	81.0	80 ± 2.5
Sagittal jaw relation ANPg (°)	−0.3	2 ± 2.5
Vertical jaw relationship		
Maxillary inclination SN^ANS-PNS (°)	8.3	8 ± 3
Mandibular inclination SN^GoGn (°)	30.1	33 ± 2.5
Vertical jaw relation ANS/PNS^GoGn (°)	21.8	25 ± 6
Dento-basal relationship		
Maxillary incisor inclination U1^ANS-PNS (°)	114.2	110 ± 6
Mandibular incisor inclination L1^GoGn (°)	85.7	94 ± 7
Mandibular incisor compensation (L1-Apo) (mm)	2.1	2 ± 2
Dental relationship		
Overjet (mm)	2.8	3.5 ± 2.5
Overbite (mm)	2.0	2.5 ± 2.5
Interincisal angle (°)	138.2	132 ± 6

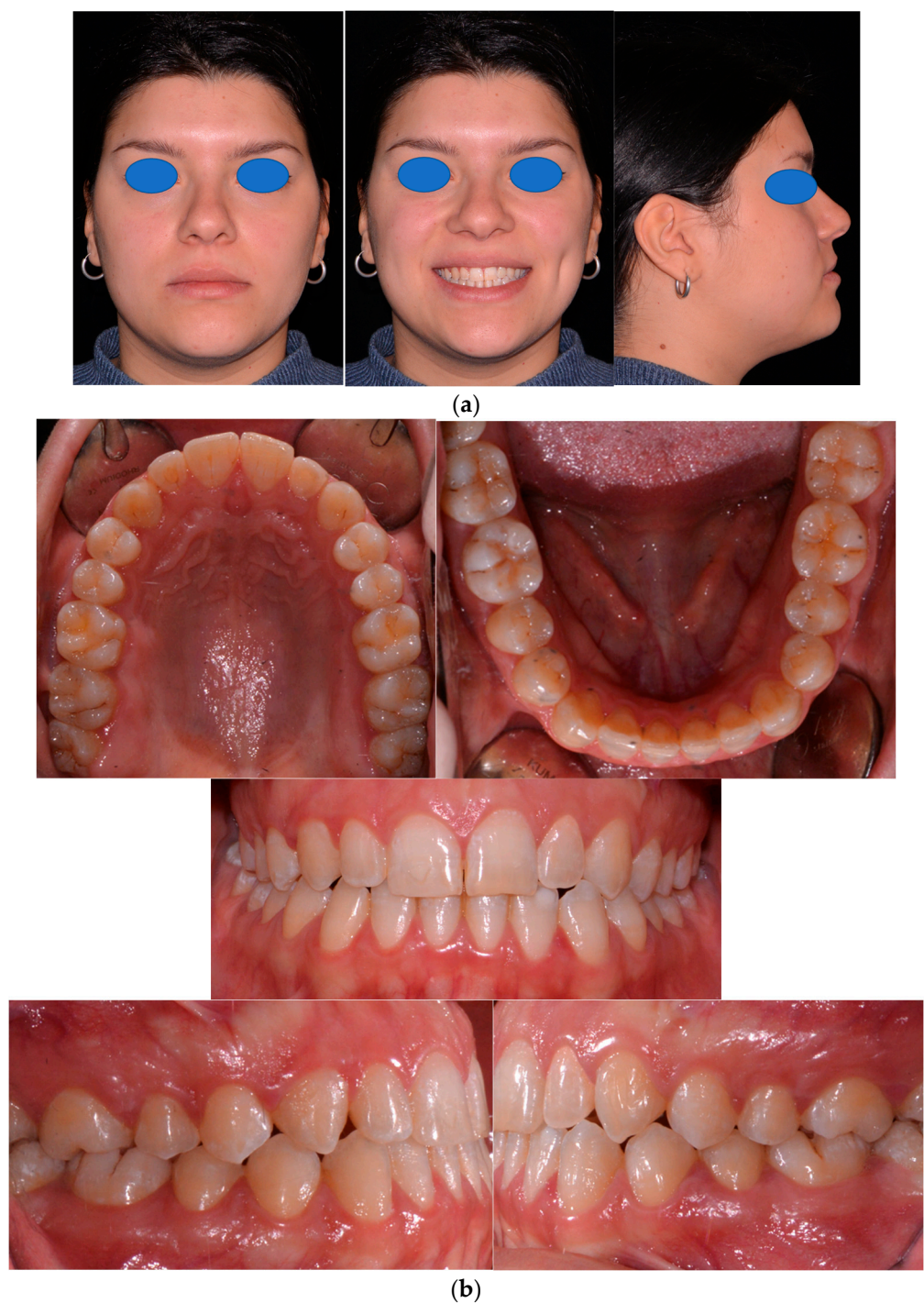


Figure 11. Patient's documentation at four-year follow-up: extraoral (a) and intraoral (b) photographs.

4. Discussion

The use of aligners might be extremely useful in the treatment of long cases such as impacted canine, considering the high prevalence of decays and TMD that can be present in some ages and the risk of demineralization due to braces [37–39]. Furthermore, to increase the predictability of the treatment, the analysis of the FEA results provided interesting information that could improve the design phase of orthodontic aligners, allowing the desired effects to be maximized and the unwanted effects to be minimized. The resulting parameters about the force system helped to compare advantages and disadvantages for each aligner configuration.

There are several studies in the literature that allow the efficiency of combinations of attachments and other auxiliaries to be evaluated depending on desired movement. Hong et al. show that the aligner with the overhanging attachment can effectively reduce crown tipping and prevent axial rotation for an intended distal displacement of the central incisor [40]. Thanks to studies that follow a similar methodology, we could state that the optimal solution for an attachment placed on the lower canine is a cylinder form attached to the lingual side of the tooth [41]. With this methodology, it is possible to evaluate the behavior of teeth not only in relation to the combination of auxiliaries, but also to the type of movement [42].

In this study, the final choice of a pre-activation point (PAP) and an attachment was justified by the numerical results obtained by FEA.

The FEA results demonstrated that the different design choices have a strong influence on the force system delivered to the tooth. The amount of Moment z (M_z) delivered to the tooth increased almost two times when adding the pressure point and the attachment to the standard aligner, while the aligner with two attachments brought a lower M_z , but also undesired lower M_x and M_y moments.

The maximum tooth displacement (0.85 mm) was gained with the pressure point and attachment aligner configuration, while the lowest (0.058 mm) was gained with the use of a couple of attachments. These results are also shown in Table 2.

Referring to Table 2, it can be noticed that the configuration led to the highest moments and forces. The double attachment instead brought load values lower than the standard aligner. The effectiveness of the choice can also be observed in Figure 9. The standard aligner does not satisfy the clinical expectations, leading to a tipping along the x -axis. With the double attachment configuration, the center of rotation (blue circle) is closer to the Cres than with the other configurations, bringing a rotation of the tooth along its long axis (z). This could probably be related to the symmetric position of the attachments with respect to the tooth's long axis. The pressure point and attachment aligner configuration generated a vestibular movement as desired by the clinician, as shown in Figure 9 and confirmed by the higher force on the vestibular direction (x -axis) compared to the other aligners.

The planning of an orthodontic aligner treatment should be split in two phases: the definition of the expected movement and the choice of auxiliary elements for each movement. Our aim was to demonstrate how the auxiliary element's features affect the interaction between the aligner and the target tooth. It was demonstrated that both an attachment and a pressure point could improve the effectiveness of the appliance. In particular, the pressure point showed a higher influence on the absolute load value.

In the scientific literature, there are studies that have investigated some clinical aspects such as the effects of distalization of the upper molars using class II elastics [43] or the comparison of the biomechanical effects of the conventional and bone-borne palatal expanders [44] with a methodology similar to that followed by us; however, there are no studies investigating the biomechanical effects of different auxiliary-aligner designs starting from a model developed on the basis of a specific patient.

However, further studies are necessary to find out more, keeping in mind the limits of this static methodology in a dynamic context such as that of the oral cavity where there are numerous variables that are difficult to reproduce (e.g., PDLs).

5. Conclusions

Computer-aided engineering (CAE) was demonstrated to be useful to analyze aligners' behaviors and provide information to enhance their design. This paper proved how CAE can improve the knowledge about tooth–appliance interactions in orthodontics. The auxiliary elements (attachment and pressure point) represent probably the most important part of the appliance since they can strongly influence the predicted outcome as shown in this study.

This optimization of the movements would constitute a series of advantages for the clinician and the patient, significantly impacting the treatment duration and avoiding

incurring a series of side effects related to orthodontic treatment like external apical root resorption (EARR), which is one of the most frequently reported iatrogenic effects of orthodontic movement [45].

According to Cattaneo et al., the use of complex and biologically coherent FEA models can help in understanding the mechanisms leading to orthodontic tooth movements as well as predicting the risk associated with specific force systems and magnitudes [46].

The method applied in the present paper should be used to analyze multiple orthodontic conditions and retrieve the best design configuration for each patient and for each specific tooth movement that needs to be planned.

Author Contributions: V.D. and T.B.; methodology, V.D., A.R., S.B. and R.S.; software, R.S.; validation, A.R., S.B. and R.S.; software, R.S.; formal analysis, R.B.; resources, V.D. and C.L.; data curation, R.S. and R.B.; writing—original draft preparation, R.B., R.S. and V.D.; writing—review and editing, R.B. and C.L.; supervision, V.D. and S.B.; patient treatment C.L. and T.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research has been supported by AirNivol S.p.A., which has supplied the materials and equipment for the clinical validation.

Institutional Review Board Statement: The study was conducted in accordance with the Declaration of Helsinki.

Informed Consent Statement: Informed consent was obtained from all subjects involved in this study.

Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

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