

Design of Customised Orthodontic Devices by Digital Imaging and CAD/FEM Modelling

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Abstract: In recent years, the public demand of less invasive orthodontic treatments has led to the development of appliances that are smaller, lower profile and more transparent with respect to conventional brackets and wires. Among aesthetic appliances, removable thermoplastic aligners gained instant appeal to patients since able to perform comprehensive orthodontic treatments without sacrificing comfort issues. The aligner must deliver an appropriate force in order to move the tooth into the expected position. However, at present, the relationship between applied force and aligner properties (i.e., aligner's thickness) is poorly understood. In this paper, a patient-specific framework has been developed to simulate orthodontic tooth movements by using aligners. In particular, a finite element model has been created in order to optimise the aligner's thickness with regard to the magnitude of the force-moment system delivered to a mandibular central incisor during bucco-lingual tipping.

1 INTRODUCTION

Orthodontic treatments are performed to achieve the correct occlusion with the best functional and aesthetic features. The correction of irregular bites is obtained by applying mechanical actions that move teeth into their proper position within the dental arches. The growing interest for adult orthodontic corrections has accelerated the use of aesthetic alternatives to conventional fixed devices. For this reason, the use of transparent tooth correction systems is becoming common for minimally invasive treatments. In particular, treatments based on clear removable thermoplastic appliances (*aligners*) are increasingly used (Boyd, 2008).

This system consists of a set of thermoformed templates, made of transparent thermoplastic material, which are sequentially worn by the patient. The orthodontic three-dimensional force-moment system on each tooth is generated by a pre-determined geometrical mismatch between the aligner shape and the dentition geometry. This condition is determined by using virtual 3D models of the patient's dentition and computer-aided design (CAD) methodologies (Beers et al., 2003). Each single template, which corresponds to the new required tooth placement, is programmed to perform only a small part of the complete tooth movement.

Therefore, a full treatment consists of a set of templates with varying shapes from the initial anatomical geometry to the target tooth position. The possibility to simulate and identify appropriate moment-to-force ratios is a key issue in order to predict and control tooth movements. At this purpose, the Finite Element Analysis (FEA) is one of the most used tools to evaluate the effectiveness of dental devices and has been widely used in dentistry since the 70's (Farah et al., 1973).

In this paper a patient-specific framework has been developed in order to make feasible a customized simulation of orthodontic tooth movements by using thermoplastic aligners. A Finite Element (FE) model is created to design optimised appliances leading to more efficient orthodontic treatments. Even if the use of aligners is becoming an effective solution to treat malocclusion conditions (Boyd, 2008), few attempts have been made to develop FE models describing the aligner's behaviour in delivering forces (Cai et al., 2015, Gomez et al., 2015).

Tooth movements with aligners may be more complex with respect to fixed appliances since there is no specific point of force application. Many parameters are certainly involved in determining the clinical outcome: tooth anatomy, aligner's material properties, amount of mismatch between aligner and dentition geometries, slipping motions between

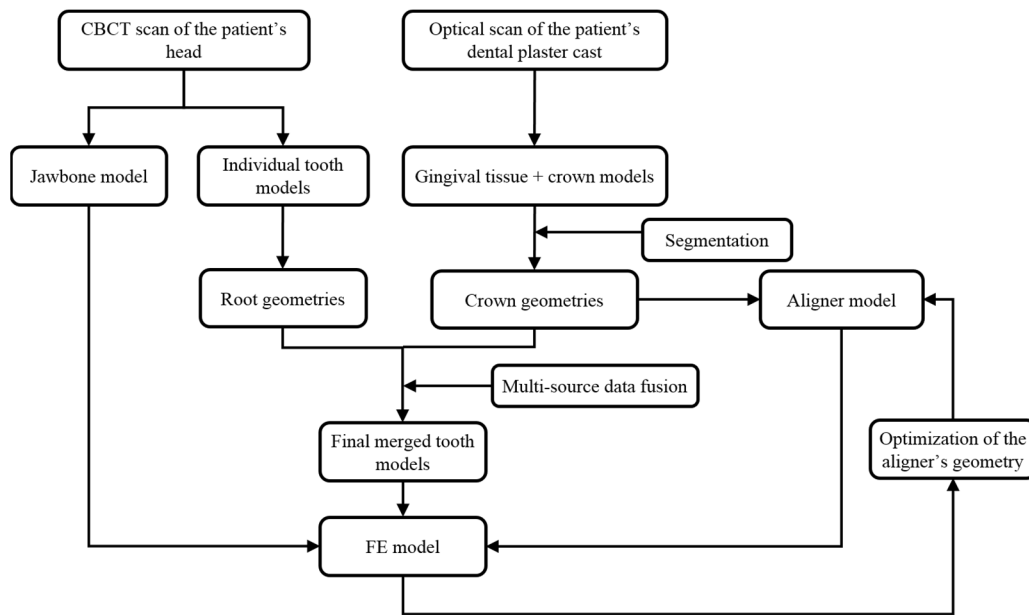


Figure 1: Overall workflow.

contact shapes. In particular, the aligner's thickness has demonstrated to have a great influence on the magnitude of the force produced by the appliance (Hahn et al., 2009, Kwon et al., 2008). In this work, the authors have used the developed FE model to study the influence of non-uniform aligner's thickness on the amount and quality of the force system delivered to a central incisor during tipping.

aligner surfaces is introduced to generate the loading condition. In particular, in this work, the influence of both thickness and shape of the aligner has been investigated in order to optimize the effectiveness of the orthodontic treatment and reduce the patient discomfort. Figure 1 summarizes the overall framework.

2 MATERIALS AND METHODS

The patient anatomical geometries as well as the aligner shape have been reconstructed by computer-aided scanning and digital imaging techniques.

In particular, multi-source data are used to obtain tooth anatomies including crown and root shapes. Ideal tooth movements can be achieved through orthodontic appliances that are designed by taking into account not only tooth crowns but also root geometrical features. For this reason, in this work, accurate crown geometries, obtained from high-precision optically scanned data, are merged with approximate representations of root geometries which are derived from a raw and fast segmentation of Cone Beam Computed Tomography (CBCT) data.

The aligner geometry has then been modelled by exploiting CAD tools in order to create a layer, which closely mates the tooth crown surfaces except for the area corresponding to the tooth to be moved. In this region, a penetration between crown and

2.1 Creation of the Patient Anatomical Model

The patient's anatomical model, composed of alveolar bone, teeth and periodontal ligament (PDL), is obtained by exploiting information derived from a CBCT patient's scan and an optical scan of the relative dental plaster cast. The CBCT scan is used to obtain complete geometries of each individual tooth along with its relative spatial arrangement within the jawbone. An optical scanner, based on a coded structured light approach, has been used to acquire the plaster model created from the patient's mouth impression. The aim of the optical scanning procedure is to reconstruct an accurate digital model composed of tooth crowns.

CBCT volumetric data are used to reconstruct the jawbone structure as well as the complete and individual tooth geometries. A CBCT scan yields a stack of slices corresponding to cross-sections through a maxillofacial volumetric region. CBCT data are stored in a sequence of Digital Imaging and Communications in Medicine (DICOM) images. An imaging slice is a 2D matrix of grey intensity values

representing the x-ray attenuation of different anatomical tissues.

The three-dimensional model of the jawbone has been obtained by exploiting tools provided by an open-source software for medical image analysis (3DSlicer, 2014). A triangular mesh of the isosurface representing the bone shape (Figure 2) has been obtained by segmenting the volumetric CBCT data set with a specific grey intensity value (isovalue).

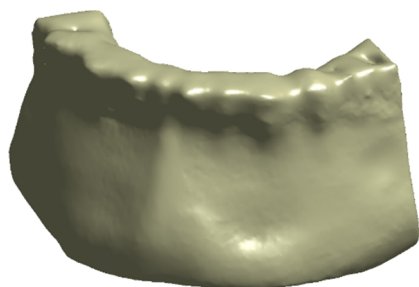


Figure 2: Jawbone geometry used in the FE model.

2.1.1 Complete Tooth Geometries by CBCT Scanning

The reconstruction of the individual tooth anatomies is not so straightforward because tooth root regions cannot be easily separated from surrounding bone tissue by only considering pixel's grey-intensity values. Most of the existing techniques are based on slice-by-slice segmentation procedures, which involve the digital processing of hundreds of slices in order to reconstruct three-dimensional geometries, thus resulting in time-consuming procedures. In this paper, DICOM images are processed by adopting the methodology introduced in (Barone et al., 2015). This method, is based on processing a small number (four) of multi-planar reformation images, which are obtained for each tooth on the basis of anatomy-driven considerations. The reformation images greatly enhance the clearness of the target tooth contours, which are then extracted and used to automatically model the overall 3D tooth shape through a B-spline representation.

Practically, four reference planar sections are automatically extracted as passing from the tooth axis and oriented along the buccolingual direction, the mesiodistal direction and the two directions disposed at 45° with respect to these two meaningful clinical views. These reference sections are used to outline the tooth by interactively tracing four different 2D tooth contours (C_i) as shown in Figure 3-a. The four contours are used to automatically extract a B-spline curve. Each slice perpendicular to

the tooth axis (transverse slice) intersect the C_i contours in eight points that are used as control points to compute a parametric B-spline curve of degree 2 (Figure 3-b). For each slice, 100 points are evaluated on the B-spline curve in order to obtain a point cloud representing the overall tooth shape. For further details the reader can refer to (Barone et al., 2015).

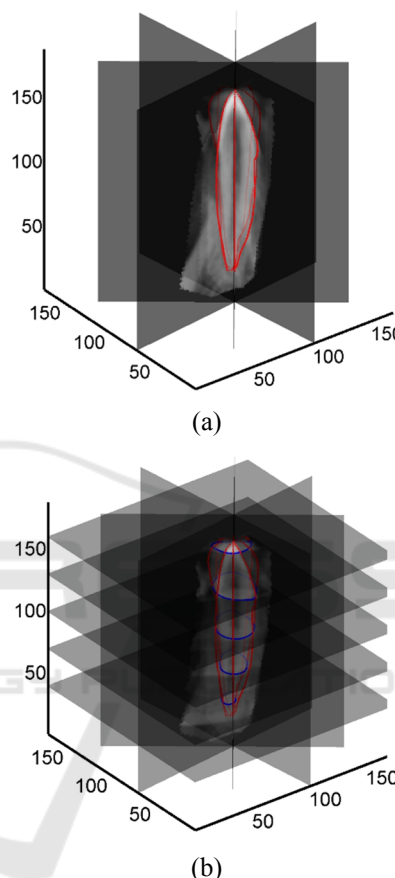


Figure 3: a) Four reference planar sections along with the 2D tooth contours, b) B-spline curves computed for the transverse slices.

Figure 4-a shows the point clouds relative to the incisors, canine and premolar teeth of the inferior arch used in the present work. Figure 4-b shows the respective StL models obtained by a tessellation of the respective point clouds.

The greatest benefit of this methodology consists in providing reliable approximations of individual tooth roots, by interactively contouring a few significant images created from the whole CBCT data set.

The processing time is greatly reduced with respect to standard cumbersome slice-by-slice methods usually proposed within medical imaging

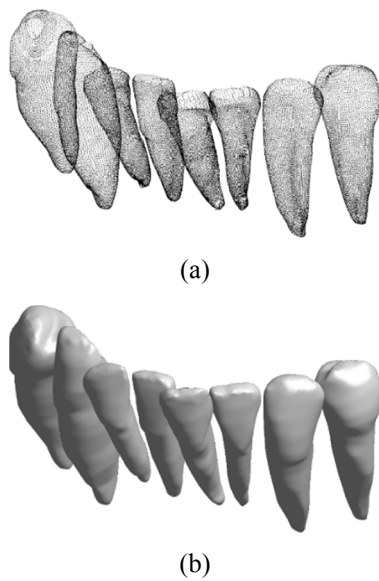


Figure 4: Incisor, canine and premolar tooth models of an inferior arch as obtained by segmenting CBCT data. (a) Point clouds, (b) STL models.

software. However, the accuracies obtained for crown geometries, especially for multi-cusped shapes, cannot be considered adequate to simulate orthodontic treatments based on the use of customized appliances.

2.1.2 Crown Geometries by Optical Scanning

In this work, an optical scanner, based on a coded structured light approach, has been used to acquire the patient's plaster model. An accurate digital mouth reconstruction composed of both crown shapes and gingival tissue is then obtained as shown in Figure 5-a. The overall surface is then segmented into disconnected regions, representing the individual crown geometries and the gingiva (Figure 5-b) through a semi-automated procedure, which exploits the curvature of the digital mouth model.

2.1.3 Multi-Source Data Fusion

For each tooth, the multi-source data obtained by using optical and tomographic scanning must be merged in order to create accurate multibody dental models. The crown surfaces obtained by optical scanning are aligned with the corresponding crown geometries segmented from the CBCT data set.

The meshes from the two sets of data are coarsely aligned into a common reference frame by manually selecting at least three common points. A refinement of the initial alignment is then

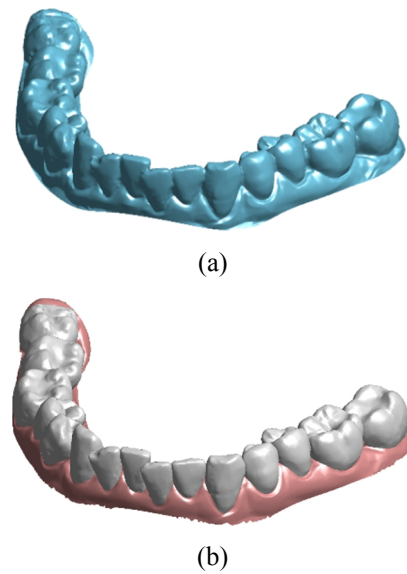


Figure 5: (a) Digital mouth model as obtained by using the structured light scanner and (b) individual tooth crowns and gingival geometries as obtained by segmenting the model.

performed by a fine registration procedure based on the Iterative Closest Point (ICP) technique. The crown geometries obtained by processing DICOM images are then removed by means of a disk vertex selection algorithm.



Figure 6: Final merged tooth geometries (optical crowns + CBCT roots) used in the FE model.

Each vertex of the optic crown is projected into a point on the CBCT mesh. This point describes the center of a sphere, which is used to select the points of the CBCT mesh to remove. The final tooth models (Figure 6) are then obtained by a Poisson surface reconstruction approach (Kazhdan et al., 2006). This allows for fully closed models composed of the most accurate representation for tooth crowns.

2.1.4 PDL Modelling

PDL geometries cannot be easily visualized and reconstructed since usually the slice thickness is

similar or even greater than the ligament space (about 0.2 mm) (Dorow et al., 2003). For this reason, in this work the PDL has been modelled for each tooth by detecting the interface area between bone and tooth models to which a 0.2 mm thick shell has been added. The volume shell is then subtracted from the alveolar bone in order to define the PDL volume (Liu et al., 2013). The obtained PDL solid models are shown in Figure 7.

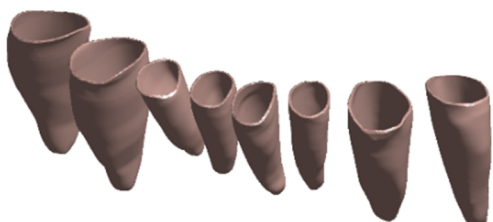


Figure 7: PDL geometries used in the FE model.

2.1.5 Orthodontic Aligner Modelling Process

The aligner geometry has been created by defining a layer completely congruent with the tooth crown surface. The individual teeth are firstly joined, root geometries are deleted and undercut volumes manually removed in order to create a unique layer. The layer is thickened to create a 0.5 mm thick volume. Finally, the merged tooth geometries (shown in Figure 6) are subtracted from the volume and the most external surface of the remaining geometry is removed with the aim at modelling the inner shape of the aligner. This procedure is carried out to guarantee an optimal fit between the mating surfaces of the tooth crowns and the appliance (Barone et al., 2014). The aligner is supposed to have a uniform 0.7 mm thickness which originates from the mean thickness of the thermoplastic material disk (0.75 mm thick) before the thermoforming process (Ryokawa et al., 2006). For this reason, a shell has been created by thickening the inner shape of the aligner by 0.7 mm along the direction normal to the surface. Figure 8 shows the overall modelled geometries used to create the FE model.

In this work, a further modelling strategy has been followed to test the influence of non-uniform aligner thickness values on the effectiveness of the orthodontic treatment. The idea is based on varying the appliance geometry by thickening the appliance in correspondence of highly deformed regions while thinning the model in correspondence of low deformed regions. This would allow to optimize the forces delivered to any tooth in the arch.

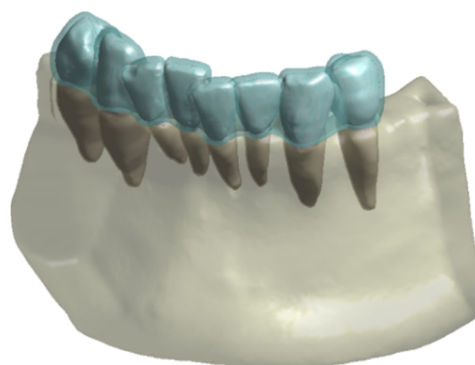


Figure 8: Overall geometries used to create the FE model.

In particular the aligner displacement values have been used to pinpoint adjust the aligner's thickness. The procedure can be schematized as follows:

1. Evaluation of the displacement value (d) for each FE mesh node of the inner surface of the 0.7 mm thick aligner;
2. Determination, for each node, of the normal direction with respect to the surface. The mean of the normal unit vectors of the triangles having that node as vertex is used;
3. Computation, for each node, of a new point along the normal direction having distance t from the node linearly defined as:

$$t = s_{\min} + \frac{(d - d_{\min})}{(d_{\max} - d_{\min})} \cdot (s_{\max} - s_{\min}) \quad (1)$$

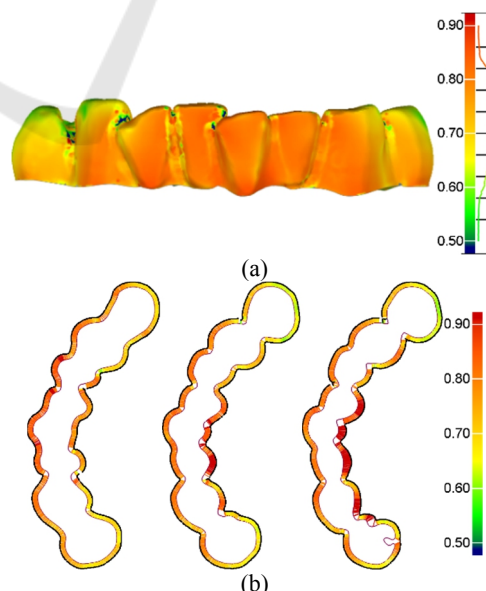


Figure 9: a) Full-field map of the aligner thickness values (expressed in mm) and three cross sections (b).

where s_{min} and s_{max} are, respectively, the minimum and maximum values which define the aligner's thickness range, while d_{min} and d_{max} respectively represent the minimum and maximum displacement values computed for the 0.7 mm thick aligner. The thickness range has been defined between 0.5 mm and 0.9 mm. Figure 9 shows a full-field map of the aligner thickness values (Figure 9-a) and three different cross sections (Figure 9-b).

2.2 Generation of the FE Model

The different bodies were imported in Ansys® 14. Each body was modeled with solid 10 nodes tetrahedrons. The approximate number of elements and nodes for each simulation was 134000 and 226000 respectively. Figure 10 shows the meshed models for the simulation performed with a uniform 0.7 mm thick aligner.

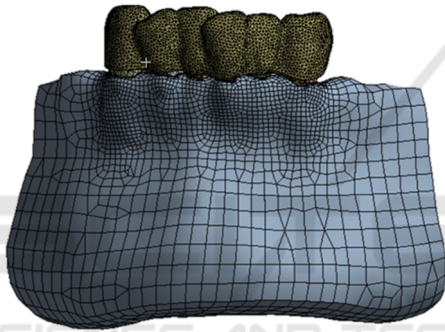


Figure 10: Meshed model used for the simulation with 0.7 mm uniform thick aligner.

2.2.1 Material Properties

A linear elastic mechanical model was assigned to each body as shown in Table 1. Moreover, teeth and bone were supposed as made by a homogenous material, without discerning in enamel, pulp, dentin for the teeth and cortical and cancellous for the bone. This simplification does not affect the simulation results as shown in previous studies (Penedo et al., 2010). In technical literature, many are the biomechanical models that simulate the tooth ligament properties (Fill et al., 2012). The investigation of the ligament in-vivo behavior is not a trivial task due to its small size (about 0.2 mm thickness). For this reason, most of the scientific literature has investigated the mechanical properties of the PDL through experimental analyses, thus developing five different models: linear elastic, bilinear elastic, viscoelastic, hyperelastic and multiphase (Fill et al., 2012). However, the complex non-linear response of the PDL does not need to be

addressed while performing an analysis about the first phase of the orthodontic reaction as in the present study (Cattaneo et al., 2005).

The thermoplastic aligners are usually made from a polyethylene terephthalate glycol-modified (PETG) disc, whose mechanical properties can be retrieved from the manufacturer's datasheet. Its mechanical behavior has been approximated as linear elastic.

Table 1: Material properties used for the FE analyses.

	Young Modulus [MPa]	Poisson's ratio
Bone	13000	0.3
Teeth	20000	0.3
PDL	0.059	0.49
Aligner (PETG)	2050	0.3

2.2.2 Loading and Boundary Conditions

A bucco-lingual tipping of a mandibular central incisor was simulated. The initial load configuration for the FE analysis was generated by the penetration between the aligner and the target tooth. The initial models do not present any penetration between teeth and aligner since the aligner is modelled onto the teeth surfaces. The tooth must be rotated around the Center of Resistance in order to create the initial penetration. The coordinates of tooth Center of Resistance were determined by using the method proposed by (Viecilli et al., 2013). The reference axes were defined accordingly to the occlusal plane. The z-axis was perpendicular to the occlusal plane, while the y and x-axis were parallel to the occlusal plane and congruent respectively with the mesiodistal and bucco-lingual tooth directions (Figure 11-a). Finally, the tooth is rotated around its C.Res. along the y-axis.

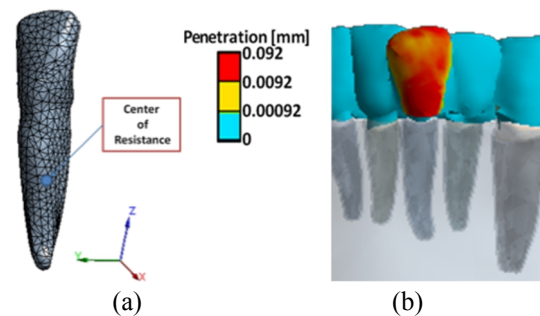


Figure 11: Target tooth's Center of Resistance (a) and initial penetration between teeth and aligner (b).

The resultant initial penetration turned out to be about 0.09 mm as shown in Figure 11-b. The bone extremities were fixed in all directions. An augmented Lagrangian formulation was used to simulate contact. Bonded contact surfaces were considered between bone and PDL and between PDL and teeth. Corresponding nodes cannot separate each other and a perfect adhesion between contact surfaces, without mutual sliding or separation, can be assumed. The aligner-teeth contact was set as frictionless, with a maximum allowed penetration of 0.01 mm which provided the best accuracy-computational time ratio. Because of the meshing process, an undesired initial penetration can occur between the aligner and the non-target teeth. For this reason the "adjust to touch" option was used for those contact couples in order to remove all the undesired initial penetrations.

2.2.3 Analysis Settings

Different scenarios were simulated to compare the influence of the aligner's thickness onto the orthodontic movement:

- uniform 0.7 mm thickness;
- uniform 0.6 mm thickness;
- non-uniform thickness (average value = 0.62 mm) obtained as described in section 2.1.5.

For each simulation, the resulting force-moment system delivered by the aligner to the target tooth was calculated at the Center of Resistance (Figure 12). Computational time resulted in about 2 hours for each simulation, using a Workstation based on Intel Xeon CPU E3-1245 v3@3.40 GHz and 16 GB RAM.

3 PRELIMINARY RESULTS

The results obtained for each scenario were analysed by comparing the moment along y-axis and the resulting moment-to-force-ratio ($M:F$) delivered to the tooth on the plane ZX (Table 2). The $M:F$ values describe the quality of the force system (Savignano et al., 2015), while M_y defines the amount of orthodontic movement. Moreover, the stress in the PDL, along the x-axis, and the tooth displacement were compared (Figure 13). The magnitude of the PDL stress values directly affects the bone remodelling process, which is the main responsible of the orthodontic movement (Penedo et al., 2010).

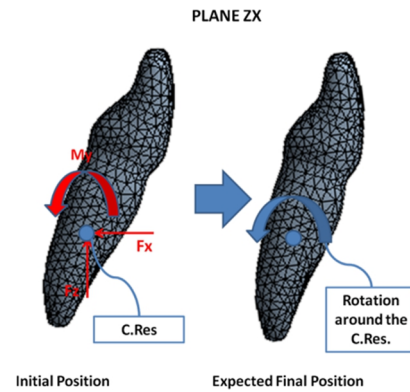


Figure 12: Initial tooth position and Force System on the plane of interest (left). Expected final tooth position (right).

Table 2: Force system delivered to the target tooth for each scenario on the plane ZX.

Aligner	0.6 mm	0.7 mm	Non-uniform
M_y [Nmm]	1.51	2.26	3.96
M_y/F_x [mm]	1.81	2.24	2.83
M_y/F_z [mm]	-2.96	-3.42	-3.06

The amount of moment delivered to the tooth increased by 50% from the 0.6 mm to the 0.7 mm thick aligner. While the non-uniform aligner elicited a moment 75% higher than the 0.7 mm and 173% higher than the 0.6 mm. The same trend was observed also for the stress values in the PDL. All different scenarios showed a positive stress value on the higher part of the anterior region and a negative stress value on the posterior, in agreement with the expected bucco-lingual movement of the tooth. The maximum stress value was almost double for the non-uniform aligner. Figure 14 shows the displacement occurring on the target tooth for the different configurations.

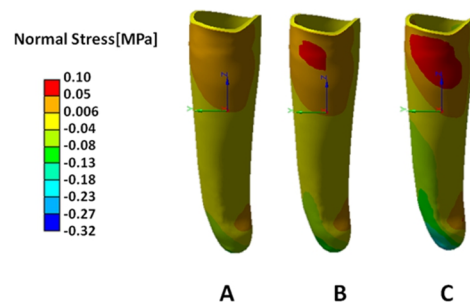


Figure 13: PDL stress values along the x-axis of the target tooth for the different simulations: A) uniform 0.6 mm, B) uniform 0.7 mm, C) non-uniform thickness.

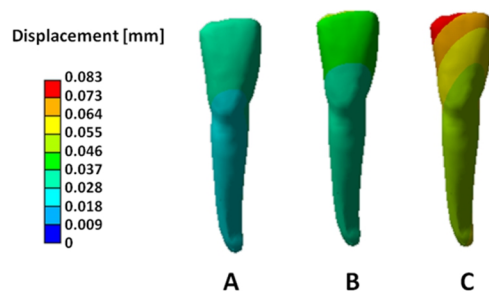


Figure 14: Displacement of the target tooth for the different simulations: A) uniform 0.6 mm, B) uniform 0.7 mm, C) non-uniform thickness.

4 DISCUSSION AND CONCLUSIONS

Thermoformed plastic aligners have demonstrated limitations in exerting complex force systems (Kravitz et al., 2009). In particular, extrusion of central incisors and rotation and inclination of canine and premolar teeth are obtained in clinical practice by using composite elements as attachments, bonded to the crowns surface, or divots and power ridges, which enhance the biomechanical effectiveness. However, the aligner thickness represents an additional critical element that should be optimized since the aligner material itself is the only element that imparts the force system. Minimal aligner thickness values would minimize patient discomfort. However, forces delivered by thick appliances are higher than those of thin materials (Hahn et al., 2009).

Typically, aligners are obtained by a vacuum thermoforming process performed onto 3D physical moulds of the teeth manufactured by RP methodologies for each single step of the orthodontic treatment. A single thermoplastic polymer resin sheet (about 0.75 mm-thick) is stretched over each prototyped mould and trimmed to extract the final configuration. For this reason, a constant thickness is usually considered for the aligners.

In this paper, the influence of non-uniform aligner's thickness for the tipping of a mandibular central incisor has been investigated by exploiting FE analyses. Preliminary results have evidenced a more effective force system delivered to the central incisor by pinpoint modulating the aligner thickness in order to vary its stiffness. The non-uniform appliance elicited a higher magnitude of the desired moment M_y and a better quality of the movement as

attested by the higher values obtained for the $M:F$ parameter.

These findings clearly call upon some considerations about the aligner's manufacturing process. Currently, the standard production processes are strictly constrained by the thermoforming procedures, which provide only constant thickness aligners. An alternative method for the direct manufacturing of the aligner should be used. For instance, milling by CNC machines or layer-by-layer printing of a single or multiple polymeric materials, would allow to obtain non-uniform thin-walled polymeric orthodontic aligners. Nevertheless, essential aligner's properties are large spring-back, high stored energy, tolerance to mouth hostile environment, biocompatibility and low surface roughness in correspondence of the mating surfaces. These features should be taken into high consideration when considering an alternative production method. This topic certainly represents a challenging task which should affect future research activities.

A further parameter that influences the effectiveness of the orthodontic treatment, besides the aligner's thickness, is represented by the mechanical properties of the thermoplastic materials. In the present study, the physical values indicated in material manufactures datasheets have been used. However, these values are given under standard atmospheric conditions. Temperature, humidity, and forming procedures may have marked effects on the actual mechanical properties, which may differ between the intraoral environment and room temperature (Ryokawa et al., 2006). For this reason, some experimental tests are currently being carried out by simulating intraoral environment in order to characterize the aligner's mechanical properties in working conditions.

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