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Consideration of root position in virtual tooth setup for extraction treatment: A comparative study of simulated and actual treatment results

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Objective: The purpose of the present study was to compare the root positions in virtual tooth setups using only crowns in a simulated treatment with those achieved in the actual treatment. **Methods:** Pre- and post-treatment intraoral and corresponding cone beam computed tomography (CBCT) scans were obtained from 15 patients who underwent orthodontic treatment with premolar extraction. A conventional virtual tooth setup was used for the treatment simulation. Pre- and post-treatment three-dimensional digital tooth models were fabricated by integrating the patients' intraoral and CBCT scans. The simulated root positions in the virtual setup were obtained by merging the crown in the virtual setup and root in the pre-treatment tooth model. The root positions of the simulated and actual post-treatment tooth models were compared. **Results:** Differences in root positions between the simulated and actual models were > 1 mm in all teeth, and statistically significant differences were observed ($p < 0.05$), except for the maxillary lateral incisors. The differences in the inter-root angulation were > 1° in all teeth, and statistically significant differences were observed in the maxillary and mandibular canines. **Conclusions:** The virtual tooth setup using only crown data showed errors over the clinical limits. The clinical application of a virtual setup using crowns and roots is necessary for accurate and precise treatment simulation, particularly in extraction treatment.

Key words: Digital models, Digital simulation, 3-dimensional diagnosis and treatment planning, Diagnosis and treatment planning

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INTRODUCTION

Accurate diagnosis and treatment planning are essential for successful orthodontic treatment. After a treatment plan is established, the study models and intraoral photographs are used for bracket positioning based on the plan; however, these data provide limited information about the position of the root. Bracket positioning should be based on Andrew's six keys of occlusion, which are in turn based on the information about the crown from the study model.[1] However, because of various crown morphology, the mesiodistal angulation and buccolingual inclination depend not only on the crown but also on the root positions.[2-7] Panoramic radiography is typically used to check the root positions; however, there are limitations. Thus, a better tool may be needed to check it more accurately.[8-12]

Treatment simulation is essential for orthodontic treatment with the extraction of permanent teeth. Conventional orthodontic setup only uses crowns. Digital technology that enables us to obtain three-dimensional (3D) models and virtual tooth setups using intraoral scans has been widely used. However, the virtual tooth setup still only uses crowns. Although ideally it would be more accurate to use both crown and root for a virtual tooth setup, there is currently no virtual tooth setup software that uses them together. For orthodontic extraction, root parallelism, root angulation, and inclination adjacent to the extraction site are critical factors for achieving excellent end-of-treatment outcomes. Therefore, it is necessary to evaluate the accuracy of a virtual setup simulation that reflects the movement of the roots. Thus, the purpose of the present study was to compare the root positions in a virtual tooth setup using only crowns in the simulated treatment with those achieved in the actual treatment. We hypothesized that there would be differences in root positions between the simulated and actual treatments.

MATERIALS AND METHODS

This retrospective study included patients with crowding or anterior protrusion who underwent conventional orthodontic treatment with premolar extraction approaches at the Chonnam National University Dental Hospital, Gwangju, Korea (CNUDH-EXP-2019-018). The inclusion criteria were as follows: (1) patients treated with upper and lower premolar extraction, (2) patients who had permanent dentitions with full clinical crown heights, (3) patients who underwent cone beam computed tomography (CBCT) and intraoral scans at both pre-treatment and post-treatment stages, and (4) patients who had proper occlusion and root parallelism at the post-treatment stage. The exclusion criteria were as follows: (1) patients with defects on the tooth surface, (2) patients requiring post-orthodontic restorative treatments, and (3) patients with incomplete pre-treatment or post-treatment records.

The sample size was calculated according to the result of a previous study by Lee et al.,[13] where the mean difference in buccolingual inclination measurements was 1.30 ± 0.92, and the effect size was calculated as 1.41. A statistical power of 80% and type 1 error of 5% were assumed using the G*power program (version 3.1.9.2; Heinrich-Heine-University, Dusseldorf, Germany). A minimum of 5 patients were needed for the study to be appropriately powered. With the inclusion and exclusion criteria, 15 consecutive orthodontic patients (4 males and 11 females) with a mean age of 18.8 ± 4.1 years were included. A total of 600 teeth (300 teeth with central and lateral incisors, canines, first or second premolars, and first molars in the pre-treatment stage; 300 teeth with central and lateral incisors, canines, first and second premolars, and first molars in the post-treatment stage) were included in the study. Thirteen patients underwent extraction of the first premolars, one patient underwent extraction of the upper right second premolar, and one patient had a missing lower left second premolar. The average treatment period was 31.1 ± 7.7 months. Of the 15 patients, seven had Class I skeletal patterns, six had Class II skeletal patterns, and two had Class III skeletal patterns (Table 1).

Table 1. Demographic data of the samples included in this study

Variables	Value
Sex (male/female)	4/11
Age (yr)	18.8 ± 4.1
ANB (°)	4.6 ± 2.8
SN/MP (°)	39.8 ± 4.9
FMA (°)	30.3 ± 4.7
FMIA (°)	51.7 ± 5.0
IMPA (°)	98.0 ± 5.9
Mx 1 to SN (°)	110.3 ± 6.3
Mx 1 to FP (mm)	15.4 ± 3.5
Mn 1 to FP (mm)	10.5 ± 2.0
UL to E-line (mm)	2.1 ± 2.4
LL to E-line (mm)	4.8 ± 2.0

Values are presented as number only or mean ± standard deviation.
ANB, A point-nasion-B point; SN/MP, sella-nasion/mandibular plane; FMA, Frankfort-mandibular plane angle; FMIA, Frankfort-mandibular incisor angle; Mx 1, maxillary incisor; Mn 1, mandibular incisor; FP, facial plane; UL, upper lip; LL, lower lip.

Intraoral and corresponding CBCT scans before and after treatment were obtained from 15 patients who had orthodontic treatment with premolar extraction. A schematic diagram to compare the virtual setup 3D tooth model and post-treatment 3D tooth model is shown in Figure 1.

The maxillary and mandibular arches were scanned using an optical intraoral scanner (TRIOS®; 3Shape, Copenhagen, Denmark) and converted into stereolithography (STL) format using the OrthoAnalyzer™ software program (3Shape). The STL data were exported to 3D reverse engineering software (Rapidform™2006; 3D Systems, Rock Hill, SC, USA). CBCT images (Alphard Vega; Asahi Roentgen, Kyoto, Japan; 80 kV and 5 mA; voxel size, 0.39 mm; and field of view, 200 mm × 179 mm) were taken. Digital imaging and communication in medicine (DICOM) files were exported to the InVivo5 software (version 5.3; Anatomage, San Jose, CA, USA) for 3D volume rendering. In the "MD (medical design) studio" module, the individual tooth including the root was segmented and converted into STL format. The CBCT crown images were separated as closely as possible from the size of the actual crown so that the locations of the roots could be accurately determined. The data for each tooth were stored separately with an ISO value of 600 for the root and 900 for the crown to obtain images of the same size as the actual teeth.

To integrate the intraoral scanned-crown images and the CBCT root images, a crown registration was performed using the 'Register' function in the software. To superimpose the images, initial registration was performed by selecting three corresponding points of the crown, and regional registration was performed based on the occlusal, buccal, and lingual surfaces of the posterior teeth and incisal, labial, and lingual surfaces of the anterior teeth. The CBCT-scanned crown image was then removed from the integrated image and replaced with an intraoral scanned crown image. After removing only the crown of the CBCT images from the superimposed images, the combined shell was used to create a 3D tooth model that combined the intraoral scanned-crown image and CBCT root image. After separating the 3D tooth model using the function of a separate cluster, an individual 3D tooth model was fabricated by splitting the crown and root shells. The pre-treatment 3D tooth model was then fabricated by merging the intraoral scanned-crown images and CBCT root images obtained at pre-treatment. Using a similar approach, post-treatment 3D tooth models were fabricated by integrating intraoral scanning and CBCT images at post-treatment.

The virtual setup for treatment simulation was performed using a pre-treatment intraoral scan in the OrthoAnalyzer program, and the simulated intraoral scan was exported to 3D reverse engineering software (Rapidform™2006) to fabricate the virtual setup 3D tooth model. The simulated intraoral scan was integrated into the pre-treatment 3D tooth model via crown registration. Initially, superimposition was approximated using a point registration function in which more than three matching points were selected on each simulated crown and its respective pre-treatment 3D tooth model crown. Gross errors after the point registration were corrected using the best-fit registration function. The pre-treatment 3D tooth model crown was then replaced with a simulated crown, and the pre-treatment tooth model crown was removed from the integrated image. The simulated tooth model was fabricated by merging the simulated crown image with the root image of the pre-treatment tooth model.

To compare the simulated and actual post-treatment tooth models, the inter-root distance, 3D root position, and angulation were measured for each tooth, including the central incisor, lateral incisor, canine, second premolar, and first molar. The surface contour of the simu-

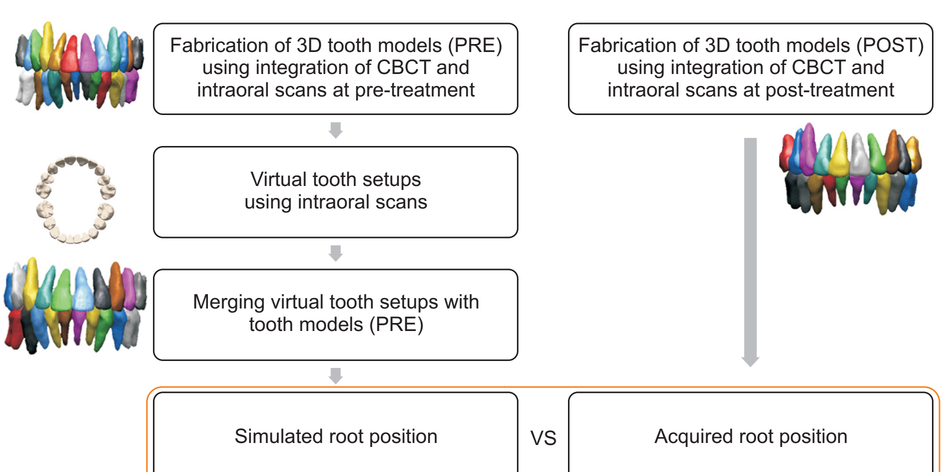

Figure 1. Application scenarios for this study. The simulated root position was compared to the actual post-treatment CBCT root position. CBCT, cone beam computed tomography; 3D, three-dimensional.

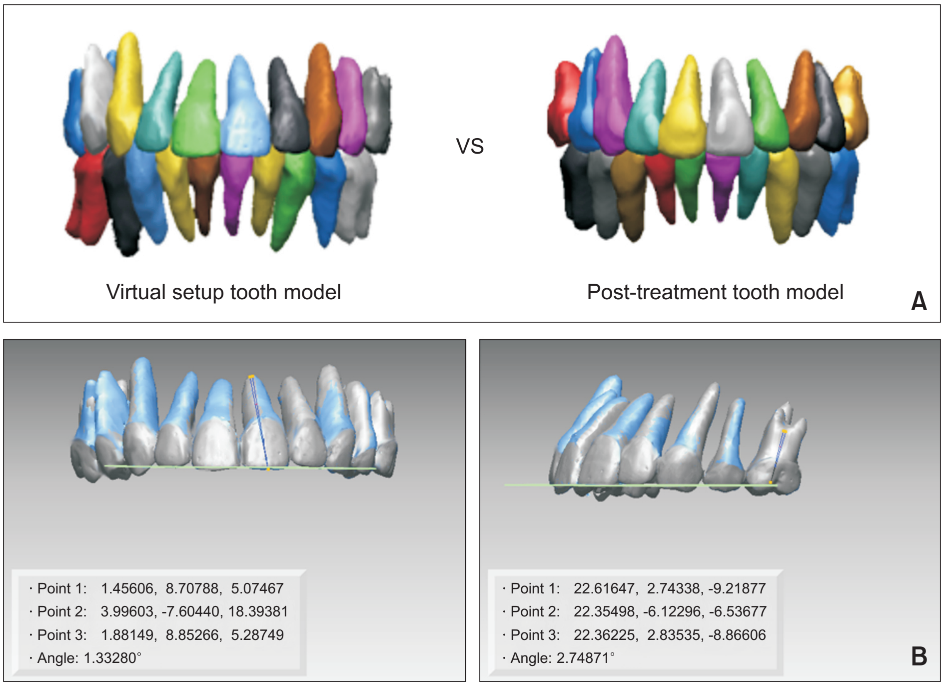

Figure 2. A, Comparison of virtual setup three-dimensional (3D) tooth model and post-treatment 3D tooth model. **B**, Measurements of 3D inter-root distance and inter-root angulation between each simulated and actual tooth model.

lated tooth model was overlaid onto the actual post-treatment tooth model using the software.

To measure the inter-root distance, the long axis of the tooth was determined by pointing to the center of the overlaid crown and each root in all three dimensions. For the incisors, canines, and premolars, a point was chosen at the end of the root. For the first molar, a point was chosen at the center of the root in the furcation area. Finally, using the three points, the root of the simulated tooth model and the actual post-treatment tooth model, and the center of the crown, the inter-root distance and inter-root angulation were measured for all teeth. The discrepancy between the simulated and actual root positions was then analyzed individually for each tooth to reduce the error caused by the morphology of the total arch (Figure 2). The investigator was trained and calibrated on how to measure the inter-root distance and angulation before collecting measurements from 15 patients.

Statistical analysis

All measurements were performed by a single investigator. The Shapiro–Wilk test was used to test the normality of the distribution of the outcome variables. The test results indicated normal distribution. Consequently, a paired sample *t*-test was used to compare the tooth positions in the simulated and actual post-treatment tooth models for each tooth. Statistical analysis was performed using SPSS version 26.0 (IBM Corp., Armonk, NY, USA). Statistical significance was set at $p < 0.05$, and all tests were two-sided. Intra-examiner repeatability was evaluated using intraclass correlation (ICC) analysis by repeating all measurements from five randomly selected individuals after 4 weeks. The ICC values ranged from 0.728 to 0.903 and 0.710 to 0.891 in the maxillary and mandibular arches, respectively.

Table 2. Comparison of inter-root distance between the simulated and actual tooth model

	Difference	*p*-value
Maxilla		
Central incisor	1.78 ± 0.61	0.031*
Lateral incisor	2.06 ± 0.73	0.091
Canine	1.84 ± 0.59	0.000***
Second premolar	2.09 ± 0.91	0.000***
First molar	1.42 ± 0.95	0.032*
Mandible		
Central incisor	1.74 ± 0.64	0.000***
Lateral incisor	2.16 ± 0.81	0.000***
Canine	2.07 ± 0.89	0.000***
Second premolar	1.96 ± 0.74	0.000***
First molar	1.01 ± 0.51	0.031*

Values are presented as mean ± standard deviation.
Data represent the distance (mm) between simulated and actual root positions at the root apex level.
*$p < 0.05$; ***$p < 0.001$ by the paired *t*-test.

RESULTS

The means and standard deviations of the absolute

Table 3. Comparison of 3-dimensional root position between the simulated and actual tooth model

	Simulated			Actual			Difference		
	X	Y	Z	X	Y	Z	X	Y	Z
Maxilla									
Central incisor	4.43 ± 2.87	11.56 ± 4.04	10.66 ± 6.13	3.75 ± 2.92	10.75 ± 4.15	10.95 ± 6.19	0.58 ± 0.79	–0.82 ± 0.91	–0.42 ± 0.99
Lateral incisor	8.81 ± 3.09	10.50 ± 4.42	9.32 ± 5.73	8.47 ± 3.10	9.95 ± 4.51	9.28 ± 6.01	0.28 ± 1.09	–0.55 ± 1.18	–0.16 ± 1.39
Canine	15.27 ± 3.91	14.31 ± 4.60	6.92 ± 4.89	14.85 ± 3.99	13.35 ± 4.40	6.77 ± 4.75	0.41 ± 0.88	–0.95 ± 1.06	0.10 ± 0.91
Second premolar	19.17 ± 4.56	11.44 ± 3.91	5.44 ± 3.38	18.49 ± 4.42	10.73 ± 4.16	4.67 ± 3.44	0.74 ± 1.27	–0.71 ± 1.10	0.71 ± 0.96
First molar	21.65 ± 5.67	5.50 ± 3.03	6.23 ± 3.84	21.30 ± 5.10	5.19 ± 3.15	6.19 ± 3.93	0.45 ± 1.06	–0.31 ± 0.98	0.21 ± 0.73
Mandible									
Central incisor	3.28 ± 2.38	22.75 ± 2.74	14.31 ± 4.75	2.98 ± 2.17	21.67 ± 2.83	14.75 ± 5.03	0.30 ± 0.72	1.08 ± 0.89	–0.43 ± 0.86
Lateral incisor	7.01 ± 2.83	23.26 ± 3.38	12.65 ± 4.90	6.59 ± 3.13	22.19 ± 3.43	12.86 ± 5.17	0.42 ± 1.09	1.07 ± 0.93	–0.21 ± 1.43
Canine	11.81 ± 3.21	25.40 ± 2.63	8.71 ± 4.41	11.44 ± 3.47	24.62 ± 2.72	9.08 ± 4.64	0.37 ± 1.05	0.78 ± 1.02	–0.38 ± 1.48
Second premolar	16.01 ± 3.88	23.54 ± 3.28	6.88 ± 3.81	15.88 ± 3.70	22.23 ± 3.47	6.95 ± 4.04	0.13 ± 0.93	1.30 ± 0.77	–0.08 ± 1.13
First molar	20.72 ± 3.25	16.33 ± 4.22	4.01 ± 3.79	20.51 ± 3.42	16.02 ± 4.08	4.10 ± 3.87	0.21 ± 0.62	0.31 ± 0.70	–0.09 ± 0.53

Values are presented as mean ± standard deviation.
The data represent the 3D distance (mm) between the simulated and actual root positions at the root apex level.
The X-, Y-, and Z-directions indicate the mediolateral, superoinferior, and anteroposterior directions, respectively. In the maxilla, positive values in the x-, y-, and z-directions indicate medial, apical, and anterior displacements, respectively; negative values in the y- and z-directions indicate occlusal, and posterior displacements, respectively. In the mandible, positive values in the x-, y-, and z-directions indicate medial, occlusal, and anterior displacements, respectively; negative value in the z-direction indicates posterior displacement.

values of the differences between the simulated and actual post-treatment tooth model measurements are presented in Tables 2 and 3. The inter-root distance between the simulated and actual tooth model in the maxilla was ≥ 1.42 mm at the maxillary first molar and ≤ 2.09 mm at the maxillary second premolar. The inter-root distance between the simulated and actual tooth model in the mandible was ≥ 1.01 mm at the mandibular first molar and ≤ 2.16 mm at the mandibular lateral incisor. The total mean differences in all measurements were 1.84 ± 0.27 mm for the maxilla and 1.79 ± 0.46 mm for the mandible. Statistically significant differences in accuracy between the simulated and actual tooth models are shown for all teeth, except the maxillary lateral incisors (Table 2).

The 3D root positions in the simulated and actual post-treatment tooth models were evaluated for each tooth. The differences were expressed by subtracting the value of the simulated tooth model from that of the actual post-treatment tooth model. A positive value on the X-axis indicated root movement in the medial direction, a positive value on the Y-axis indicated movement in the root direction in the maxilla and movement in the occlusal direction in the mandible, and a positive value on the Z-axis indicated root movement in the forward direction. When comparing the roots of the simulated and actual tooth models, the simulated roots were located in the lateral and occlusal directions compared to the actual roots in both the maxilla and mandible, and the Z-axis values were inconsistent (Table 3).

Percentage differences in values outside the clinically acceptable range of ± 2.5° were observed in the maxillary central incisor, lateral incisor, mandibular central incisor, lateral incisor, and canine. The means and standard deviations of the differences in the inter-root angulation between the simulated and actual post-treatment tooth models are shown in Table 4. The inter-root angulation between the simulated and actual tooth models in the maxilla was ≥ 1.25° at the maxillary second premolar and ≤ 3.21° at the maxillary central incisor. The inter-root angulation between the simulated and actual tooth model in the mandible was ≥ 1.40° at the mandibular second premolar and ≤ 2.88° at the mandibular canine. The total mean difference in all measurements was 2.15 ± 0.89° in the maxilla and 2.23 ± 0.73° in the mandible. However, inter-root angulation differences between the simulated and actual tooth models were statistically significant in the maxillary canine ($p < 0.05$) and mandibular canine ($p < 0.01$) adjacent to the extraction site.

DISCUSSION

Root position and root parallelism are important factors for successful orthodontic treatment. Therefore, accurate bracket positioning is necessary. Currently, root position is primarily evaluated according to panoramic radiographs, and the American Board of Orthodontics recommends evaluation of root angulation using panoramic radiographs; however, these often contain distortions, resulting in an inaccurate portrayal of root angulations.[14] Although the introduction of CBCT has been helpful in orthodontics by enabling 3D positioning of the roots, based on the ALARA (As Low As Reasonably Achievable) principle the root position should not be replaced by CBCT if it is sufficiently understood by the study model or panorama alone.[15]

Table 4. Difference of inter-root angulation between the simulated and actual tooth model

	Simulated	Actual	Difference	*p*-value
Maxilla				
Central incisor	85.40 ± 18.11	85.88 ± 25.38	3.21 ± 2.21	0.514
Lateral incisor	82.83 ± 32.17	83.35 ± 26.19	2.99 ± 2.56	0.468
Canine	74.43 ± 21.04	75.27 ± 18.87	1.78 ± 1.50	0.046*
Second premolar	82.63 ± 19.77	82.14 ± 19.22	1.25 ± 1.09	0.107
First molar	82.76 ± 24.03	82.63 ± 20.42	1.51 ± 1.19	0.717
Mandible				
Central incisor	84.73 ± 35.67	86.23 ± 10.10	2.83 ± 3.19	0.051
Lateral incisor	85.83 ± 13.17	86.54 ± 05.29	2.55 ± 2.13	0.243
Canine	75.74 ± 31.74	77.83 ± 30.95	2.88 ± 2.42	0.001**
Second premolar	81.36 ± 23.43	81.05 ± 18.14	1.40 ± 1.28	0.371
First molar	79.33 ± 23.14	79.50 ± 22.29	1.49 ± 0.89	0.601

Values are presented as mean ± standard deviation.
The data are presented as degrees (°) between the simulated and actual root axes at the extraction site.
*$p < 0.05$; **$p < 0.01$ by the paired t-test.

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However, even scans with accurate crown data do not show the root position accurately, and CBCT has a limitation in that it does not represent the occlusal surface in detail; therefore, several studies have merged crown images and CBCT root images for virtual setup.[16-21] Macchi et al.[16] presented a method for establishing a treatment plan that considers the location of the root before orthodontic treatment by composing the laser-scanned image with the CBCT root image. Kihara et al.[18] and Lightheart et al.[19] synthesized laser-scanned crowns using CBCT root images and revealed the accuracy of the tooth model that visualized the 3D root position. Lee et al.[20,21] showed that the 3D root position could be determined during or after orthodontic treatment using laser-scanned crown images and CBCT images. Grünheid et al.[22] evaluated the accuracy of a virtual setup for Invisalign using surface-based registration in nonextraction cases. They compared a post-treatment model and virtual treatment plan model; however, in their virtual tooth setup, only the tooth crown images were used. In orthodontic treatments with extraction, simulating the root position during virtual tooth setup is necessary to predict root movement.

In the present study, the virtual setup model was derived from software simulations using only the crown images. Thus, the crown position in the simulation would be different from that in the actual post-treatment stage. By integrating the simulated crown images and pre-treatment tooth model, the resulting root position would be different from that of the actual post-treatment tooth model. This study aimed to compare the root positions in a virtual tooth setup using only crowns in simulated treatment with those achieved in actual treatment. In the comparison between the simulated and actual post-treatment tooth models, the values of the maxillary and mandibular incisors tended to be slightly greater than those of the other teeth. In particular, the difference in the anterior teeth was thought to be due to prominent root resorption in the incisors after orthodontic treatment, especially compared with the pre-treatment stage. In addition, other factors can cause differences in root size and shape, such as noise, voxel size, contrast variance, and segmentation accuracy. A potential solution for this would be to use low-dose spiral CT rather than CBCT, as the former has been shown to generate high-quality images for orthodontic diagnosis without a significant increase in radiation for patients.[23]

Inter-root angulation measurements in the simulated and actual post-treatment tooth models showed a difference of > 1° in all teeth. In particular, there was a difference of > 2° in the maxillary and mandibular anterior teeth, and significant differences were observed in the maxillary and mandibular canines. This was because it was difficult to distinguish the root axes in these cases. Measuring the root axis involves comparing the angular difference by marking the crown and the root apex; it was difficult to accurately measure the root axis in such cases. It is also apparent that positioning the bracket using the crown image alone does not accurately reflect the root location if the incisal edge of the anterior tooth does not have an ideal crown shape due to attrition or an abnormal form. The methodology used in the present study to measure inter-root distance and inter-root angulation has been used in previous studies.[24,25] Based on the repeatability of measurements, the repeatability was found to be clinically acceptable (ICC values were 0.728–0.903 and 0.710–0.891 in the maxillary and mandibular arches, respectively).

In this study, there was a significant difference between each measurement when a virtual setup was prepared without any information regarding the crown or post-treatment. This indicates that a virtual setup using crown images alone does not reflect 100% of the actual root position, and a digital bracketing setup using intraoral scans that does not consider the root position also has practical limitations. Moreover, there were some technical limitations. No program combines CBCT root images and intraoral scans, and the process of making 3D tooth models is time-consuming. Furthermore, because of the large size of the datasets, including the roots of the entire dentition, a high capacity of computation is required to run the software using crown and root data simultaneously. However, these shortcomings could be overcome through future technological advances. Therefore, there is a need to develop a new virtual setup program that can simulate the root position during the integration of crown information. The present study has some limitations owing to its retrospective design. For example, a true cause-and-effect relationship cannot be established definitively through retrospective studies. Nevertheless, our study provides valuable findings that could serve as a benchmark for future prospective studies in this field.

CONCLUSIONS

The study demonstrated that compared to the actual post-treatment tooth model, the simulated tooth model from a virtual setup using only the crown did not fully consider root positioning in bracket positioning. Therefore, a virtual setup using crown and root data should be implemented in clinical practice for accurate and precise treatment simulations.

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AUTHOR CONTRIBUTIONS

Conceptualization: KCL. Data curation: MP. Formal analysis: MP. Funding acquisition: KCL. Methodology: KCL. Project administration: KCL. Visualization: MP. Writing–original draft: MP, KCL. Writing–review & editing: VA, PA, MKL, KCL.

CONFLICTS OF INTEREST

No potential conflict of interest relevant to this article was reported.

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