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Effect of auxiliary lever arm angulation and elastic type on mandibular molar mesialization with clear aligners: a three-dimensional finite element analysis

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Abstract

Background Mesialization of a mandibular second molar into a first molar extraction site is among the least predictable movements in clear aligner therapy, because force delivered at crown level generates a moment about the centre of resistance. Auxiliary lever arms and elastics move the force vector apically, but the combined influence of lever arm angulation and elastic type has not been quantified.

Methods Ten three-dimensional finite element models of a mandible with a missing first molar were built from cone-beam computed tomography data. Each included a 0.5 mm aligner, an attachment, a miniscrew and, where applicable, a button or a lever arm angulated 0°, 30° mesially or 30° distally to the molar long axis, with intramaxillary or Class II intermaxillary elastics. A single 0.25 mm activation with 1.5 N was simulated. Displacement of four cusp tips and two root apices was recorded along three axes, and for each axis the net displacement (translation) and the crown–root difference (rotation) were calculated separately. Von Mises stresses in the periodontal ligament were recorded.

Results Mesial tipping predominated, being greatest with a buccal button and Class II elastics ($\Delta X -0.158 \mu\text{m}$) and smallest with a lever arm angulated 30° distally plus an intramaxillary elastic ($\Delta X -0.002 \mu\text{m}$). Net mesial translation was greatest in the two configurations that produced mesial root tipping (-0.039 and $-0.042 \mu\text{m}$). Vertical direction depended solely on elastic type: every Class II configuration extruded the molar and every intramaxillary configuration intruded it. The vertical crown–root difference correlated inversely with the transverse one ($r = -0.98$) but only weakly with the sagittal one ($r = -0.18$), indicating that it reflects transverse rather than vertical rotation. Peak von Mises stress correlated only moderately with total displacement ($\rho = 0.65$).

Conclusions Elastic type appears to govern the vertical direction of molar movement, whereas the angulation of the lever arm governs the magnitude and direction of tipping. A lever arm angulated 30° distally combined with an intramaxillary elastic gave the lowest tipping, the lowest total displacement and the lowest periodontal ligament stress, and is considered the most balanced of the configurations examined.

Keywords

Finite element analysis; Clear aligner; Molar mesialization; Lever arm; Intermaxillary elastics; Periodontal ligament; Biomechanics; Tooth movement

Background

Clear aligners are removable, patient-specific appliances manufactured from thermoplastic materials that move teeth gradually towards a targeted position. Unlike fixed appliances, the orthodontic force in aligner therapy arises from the elastic recovery of the deformed thermoplastic shell rather than from a pulling element [1]. Predicting the direction and magnitude of the force generated by an aligner is therefore central to treatment success [2]. For certain movements, however, clinical predictability remains low. Mesialization of a

mandibular molar is among the least predictable, as mesial tipping and rotation of the molar are frequently reported [3, 4].

The permanent mandibular first molar is the tooth most commonly lost [16]. Closing the resulting extraction space by mesializing the second molar removes the need for prosthetic restoration and preserves alveolar bone [4, 17]. Fixed appliances combined with skeletal anchorage can achieve this movement predictably [18], but the biomechanical behaviour of the same mechanics within an aligner system is not fully understood.

Applying force closer to the centre of resistance reduces tipping and produces more controlled movement [19, 20]. Auxiliary lever arms are used for this purpose, transferring the point of force application apically [22]. Elastics, used as removable force elements since the nineteenth century for the correction of sagittal, vertical and transverse discrepancies [6-9], provide the force. Elastics are inexpensive and versatile, but require patient compliance and may generate unwanted rotation or extrusion when applied incorrectly [10, 11]. The position and angulation of an auxiliary element alter the sagittal, vertical and transverse components of the force vector and therefore the moment-to-force ratio acting on the tooth [9, 24].

Finite element analysis (FEA) allows stresses and displacements arising from a defined force system to be computed for structures with irregular geometry and heterogeneous material properties [12]. It is widely applied in aligner biomechanics because it gives access to quantities that cannot be measured clinically [13-15].

A previous iterative finite element study examined the cumulative biomechanical effect of auxiliary devices during mandibular molar mesialization with aligners [2]. To our knowledge, however, no study has evaluated how the angulation of a prefabricated auxiliary lever arm relative to the long axis of the tooth interacts with the method of elastic application (intramaxillary or Class II intermaxillary) to determine three-dimensional tooth movement and periodontal stress. The present study was designed to identify the auxiliary configuration

and force vector that minimize unwanted movement during mandibular molar mesialization with clear aligners.

Methods

Ethical approval

Ethical approval was obtained from the Hamidiye Scientific Research Ethics Committee of the University of Health Sciences (approval number 24/584, dated 20 September 2024). The study used an anonymized archival cone-beam computed tomography (CBCT) data set and involved no prospective intervention on human participants.

Cone-beam computed tomography acquisition

Geometric models of the mandible were constructed from a CBCT scan of an adult patient, obtained from the archive of Ay Tasarım Ltd (Ankara, Türkiye). Scanning was performed with an ILUMA unit (Orthocad CBCT, 3M Imtec, Oklahoma, USA) at 120 kVp and 3.8 mA for 40 s, yielding 601 slices.

Modelling procedure

The reconstructed slices were saved in DICOM 3.0 format and imported into 3D-Doctor (Able Software Corp., Lexington, MA, USA). Bone tissue was isolated by interactive segmentation and a three-dimensional model of the mandible was generated with the 3D Complex Render technique. Surface simplification tools were used to obtain a smooth mesh of uniformly proportioned elements, and the model was exported in stereolithography (.stl) format.

A cortical bone shell was created by applying a 2 mm offset to the mandibular model, and trabecular bone was generated from the inner surface of this shell. The mandibular teeth were modelled as homogeneous structures without differentiating enamel from dentine. After the

teeth were positioned within the bone, the root surfaces below the alveolar crest were extracted and a periodontal ligament (PDL) of uniform 0.25 mm thickness was created. A clear aligner 0.5 mm thick was designed over the anatomical crowns.

A rectangular attachment measuring $3 \times 2 \times 1$ mm was designed on the mandibular second molar (MM2) targeted for mesialization, placed vertically at the midpoint of the distal aspect of the clinical crown and positioned buccally or lingually according to the direction of the planned force. An orthodontic button was designed with a 3 mm mesh base, a 1 mm neck and a 2 mm head. The lever arm was designed with a 3 mm mesh base, a 6 mm arm length and a 1 mm cross-sectional diameter. Buttons and lever arms were positioned at the midpoint of the clinical crown. Miniscrews measuring 1.6×8 mm provided skeletal anchorage. Models were assembled in ANSYS SpaceClaim (ANSYS Inc., Canonsburg, PA, USA) and the mandibular first molar was removed to represent the extraction site.

Coordinate system

A Cartesian coordinate system was established to describe three-dimensional displacement. The X-axis represents the sagittal plane, with positive values indicating distal and negative values mesial movement. The Y-axis represents the vertical plane, with positive values indicating extrusion and negative values intrusion. The Z-axis represents the transverse plane, with positive values indicating lingual and negative values buccal movement.

Material properties and boundary conditions

Meshes were built predominantly from eight-node brick solid elements; elements with fewer nodes were used where required to complete the geometry. Node and element counts for each model are given in Table 1. All tissues and materials were assumed to be linear, homogeneous and isotropic. Young's moduli and Poisson's ratios were taken from published data [2] and are listed in Table 2. The inferior and posterior nodes of the mandible were constrained in all

degrees of freedom. Bonded contact was defined between interfacing surfaces, and a surface-to-surface contact with a Coulomb friction coefficient of 0.2 was assigned between the aligner, the teeth and the attachments.

Loading method

A two-step loading procedure was used. The MM2 was first displaced 0.25 mm, and the resulting deformation of the aligner was computed in ANSYS (ANSYS Inc., Canonsburg, PA, USA). The reaction forces produced by this deformation were then applied to the corresponding teeth in the reverse direction. In the scenarios employing auxiliary elements, an elastic force of 1.5 N was applied in addition to the aligner-derived force.

Experimental design

Ten configurations were modelled (Table 1). Scenario 1 used the aligner alone. Scenario 2 used a mid-buccal button with a Class II intermaxillary elastic anchored to a maxillary miniscrew. Scenario 3 used a mid-buccal button with an intramaxillary elastic anchored to a mandibular miniscrew. Scenario 4 used a mesiolingual button with a Class II intermaxillary elastic anchored to a palatal miniscrew. Scenarios 5 to 7 used Class II intermaxillary elastic anchored to a maxillary miniscrew, the arm being parallel to the long axis (Scenario 5), angulated 30° mesially (Scenario 6) or 30° distally (Scenario 7). Scenarios 8 to 10 used the same three lever arm positions with an intramaxillary elastic anchored to a mandibular miniscrew.

Evaluation of tooth movement

Six landmarks were selected on the MM2: the mesiobuccal (MBCT), mesiolingual (MLCT), distobuccal (DBCT) and distolingual (DLCT) cusp tips, and the mesial (MRA) and distal

(DRA) root apices. Crown displacement was defined as the mean displacement of the four cusp tips and root displacement as the mean displacement of the two apices.

Because a tooth is approximately 27,000 times stiffer than the PDL (18,600 MPa against 0.68 MPa), it behaves as a rigid body under the loads applied here, and its movement can be decomposed into a translational and a rotational component. Two quantities were therefore calculated for every axis. The net displacement, representing translation, was obtained as the mean of the crown and root values, and the crown–root difference, representing rotation, was obtained as crown minus root:

$$\text{Net} = (\text{Crown} + \text{Root}) / 2$$

$$\Delta = \text{Crown} - \text{Root}$$

For the X and Z axes the distance between the crown landmarks and the apices is perpendicular to the direction of movement, so the crown–root difference reflects a genuine moment arm and quantifies mesiodistal and buccolingual tipping respectively. Negative ΔX indicates mesial tipping and positive ΔX distal tipping; positive ΔZ indicates lingual crown tipping and negative ΔZ buccal crown tipping. For the Y axis the crown landmarks and the apices lie approximately on the same vertical line, so no comparable moment arm exists and the crown–root difference cannot be interpreted as intrusion or extrusion. Vertical movement was therefore evaluated from the net vertical displacement, with negative values indicating intrusion and positive values extrusion.

Statistical analysis

Finite element analysis is deterministic and produces a single solution for each model, so inferential statistics were not applicable [22]. Relationships between the computed quantities were quantified descriptively, using the Pearson correlation coefficient for linear associations

between displacement components and the Spearman rank correlation coefficient for the association between displacement magnitude and peak stress.

Use of large language models

A large language model (Claude, Anthropic) was used to cross-check the arithmetic consistency of the tabulated displacement values, to compute the derived quantities reported in Tables 4 to 7, and to assist with language editing. The authors verified all numerical results against the solver output and take full responsibility for the content of the manuscript.

Results

Sagittal (X-axis) movement

Displacements of the six landmarks are given in Table 3 and illustrated in Fig. 1. Net sagittal displacement and the crown–root difference are given in Table 4 and Fig. 2.

The crown–root difference was negative in eight of the ten scenarios, indicating that mesial tipping was the dominant tendency. Tipping was greatest in Scenario 2 ($-0.158347\ \mu\text{m}$), Scenario 5 ($-0.147282\ \mu\text{m}$) and Scenario 6 ($-0.145147\ \mu\text{m}$), the three configurations in which force was delivered from the buccal surface with a Class II elastic. The smallest values were recorded in Scenario 10 ($-0.001793\ \mu\text{m}$) and Scenario 4 ($-0.006527\ \mu\text{m}$).

Net sagittal displacement showed a different ranking. Scenario 9 ($-0.042145\ \mu\text{m}$) and Scenario 8 ($-0.039143\ \mu\text{m}$) produced the largest net mesial movement of the tooth as a body, followed by Scenario 4 ($-0.017783\ \mu\text{m}$) and Scenario 10 ($-0.011402\ \mu\text{m}$). These two scenarios were also the only ones with a positive crown–root difference, indicating that the apices moved further mesially than the crown and that mesial root tipping occurred. In Scenario 1 ($-0.000890\ \mu\text{m}$) and Scenario 3 ($-0.001050\ \mu\text{m}$) both the crown–root difference

and the net displacement were very small, indicating that the tooth neither tipped appreciably nor advanced.

Vertical (Y-axis) movement

Vertical displacements of the six landmarks are given in Table 3 and illustrated in Fig. 3. Net vertical displacement and the crown–root difference are given in Table 5 and Fig. 4.

Net vertical displacement was negative, indicating intrusion, in Scenarios 1, 3, 8, 9 and 10, and positive, indicating extrusion, in Scenarios 2, 4, 5, 6 and 7. This division corresponded exactly to the type of elastic used: extrusion occurred in every scenario with a Class II intermaxillary elastic and intrusion in every scenario with an intramaxillary elastic. In Scenario 1, where no auxiliary element was used, a small intrusive displacement was recorded ($-0.005186 \mu\text{m}$). The largest intrusion was seen in Scenario 3 ($-0.063795 \mu\text{m}$) and the largest extrusion in Scenario 6 ($+0.051761 \mu\text{m}$). Vertical displacement was smallest in Scenario 1 and Scenario 10 ($-0.008083 \mu\text{m}$).

The vertical crown–root difference did not follow the same pattern as net vertical displacement. Across the ten scenarios it correlated strongly and inversely with the transverse crown–root difference ($r = -0.98$) but only weakly with the sagittal one ($r = -0.18$); the signs of ΔY and ΔZ were opposite in all ten scenarios (Fig. 9). The vertical crown–root difference therefore represents the vertical projection of buccolingual tipping rather than an independent vertical movement.

Transverse (Z-axis) movement

Transverse displacements of the six landmarks are given in Table 3 and illustrated in Fig. 5. Net transverse displacement and the crown–root difference are given in Table 6 and Fig. 6.

The crown–root difference was positive in eight scenarios, indicating lingual crown tipping. It was greatest in Scenario 3 (+1.093275 μm), a value 2.6 times that of the next highest scenario and 20 times that of the lowest. Scenarios 5 (–0.287045 μm) and 6 (–0.412750 μm) were the exceptions, both showing buccal crown tipping with the crown moving buccally and the apices lingually. These were the two configurations combining a buccal lever arm with a Class II elastic anchored in the maxilla. Transverse tipping was smallest in Scenario 7 (+0.053125 μm), Scenario 10 (+0.063095 μm) and Scenario 1 (+0.088370 μm).

Net transverse displacement was largest in Scenario 6 (+0.080925 μm) and Scenario 5 (+0.067078 μm), where apical movement exceeded coronal movement approximately threefold, so that the tooth as a body shifted lingually while the crown tipped buccally.

Total displacement and periodontal ligament stress

Mean total displacement of the six landmarks and von Mises stresses in the PDL are given in Table 7; stress distributions are shown in Fig. 7 and stress magnitudes in Fig. 8.

Total displacement was greatest in Scenario 3 (0.56568 μm), 2.6 times the value of the next highest scenario, and smallest in Scenario 10 (0.03386 μm) and Scenario 7 (0.03513 μm). In Scenario 3, however, net sagittal displacement was only –0.001050 μm , so almost all of the movement was expended on transverse tipping and vertical intrusion rather than on mesial advancement.

Maximum von Mises stress was highest in Scenario 8 (8.3032 kPa), followed by Scenario 6 (8.000 kPa) and Scenario 9 (7.0836 kPa), and lowest in Scenario 10 (0.4643 kPa) and Scenario 7 (0.9109 kPa). Minimum von Mises stress was highest in Scenario 3 (0.010870 kPa) and lowest in Scenario 10 (0.000689 kPa). The rank correlation between mean total displacement and maximum von Mises stress was moderate ($\rho = 0.65$). Two scenarios departed from the general trend: Scenario 8 had the fourth lowest total displacement but the

highest peak stress, whereas Scenario 3 had the highest total displacement but only the fourth highest peak stress.

Discussion

Loss of the permanent mandibular first molar is common [16], and closing the extraction space by mesializing the second molar avoids prosthetic restoration [4, 17]. Although auxiliary elements such as buttons, attachments, miniscrews and elastics have widened the range of malocclusions treatable with aligners [5], the success rate of molar mesialization remains low and unwanted mesial tipping and rotation are frequently reported [3, 4]. The biomechanical behaviour of these auxiliaries within an aligner system is not yet fully described [23].

The present findings suggest that tooth movement is not adequately characterized by a single quantity. Since the tooth behaves essentially as a rigid body under the loads applied, its displacement can be decomposed into a translational and a rotational component, and it appears preferable for these two components to be reported separately. Scenarios 1 and 3 illustrate this point. Both showed small crown–root differences along the sagittal axis (-0.012112 and -0.021353 μm), which in isolation might suggest controlled movement; their net sagittal displacements, however, were -0.000890 and -0.001050 μm , indicating that the tooth neither tipped appreciably nor advanced to a meaningful extent. Scenario 10, by contrast, combined the smallest crown–root difference of the series with a net displacement more than ten times greater. A low crown–root difference therefore appears to be a necessary but not a sufficient indicator of controlled tooth movement. Yang et al. [25], who examined the influence of aligner anchorage preparation on mandibular first molars during premolar-

extraction space closure, likewise evaluated molar behaviour in three dimensions rather than through a single displacement value.

Force applied at crown level acts at a distance from the centre of resistance, which in mandibular molars lies close to the furcation [19], and the resulting moment tips the crown mesially [18]. Moving the point of force application closer to the centre of resistance reduces this moment [20], and our data are consistent with that principle: the crown–root difference was smaller in the lever arm scenarios than in the button scenarios employing the same elastic. The angulation of the lever arm was as influential as its presence. Within both elastic groups, distal angulation was associated with the lowest tipping (Scenario 7 among the intermaxillary configurations and Scenario 10 among the intramaxillary ones), which suggests that displacing the force vector distal to the centre of resistance generates a counter-moment opposing mesial tipping. İnan and Gonca [24] reported that the length and material of a power arm influenced canine displacement and periodontal ligament stress in aligner therapy, and the present findings suggest that a comparable relationship may hold for molar mesialization.

Scenario 4, in which a mesiolingual button was combined with a Class II elastic anchored to a palatal miniscrew, is of interest in this respect. Although no lever arm was used, this configuration produced the second lowest sagittal crown–root difference of the series ($-0.006527\ \mu\text{m}$) together with the third largest net mesial displacement ($-0.017784\ \mu\text{m}$). This pattern is consistent with the observations of Wang et al. [26], who recommended a mesiolingual elastic together with a distolingual attachment in order to minimize mesial tipping during Class II elastic application with clear aligners. Lingual positioning of the point of force application may therefore offer an alternative means of limiting sagittal tipping where a lever arm is not desirable, although the transverse consequences of this configuration should also be taken into account.

Scenarios 8 and 9 behaved differently from the remaining configurations, the apices moving further mesially than the crown and producing mesial root tipping. These two configurations also generated the largest net mesial displacement of the series. Nagaraj et al. [18] described a comparable root-first pattern during miniscrew-anchored protraction of mandibular second molars, and Morita et al. [23] noted that similar biomechanical considerations apply when impacted mandibular molars are uprighted. This pattern may be advantageous where root paralleling is the objective, although in Scenario 8 it was accompanied by the highest peak von Mises stress recorded in the present study, which may be relevant when the risk of root resorption is considered [31, 32].

Vertical behaviour was governed by the type of elastic in all ten configurations. Aligners worn for 20 to 22 hours a day are considered to exert a bite-block effect that intrudes posterior teeth [28], and the small intrusive displacement recorded in Scenario 1, where no auxiliary element was used, is consistent with this. The extrusive vertical component of a Class II elastic acts against that effect, and in every Class II scenario it prevailed, resulting in net extrusion; the intrusive component of an intramaxillary elastic acts in the same direction, and in every intramaxillary scenario intrusion was observed. Class II elastics are known to introduce substantial vertical and transverse force components [9], and Wang et al. [26] reported a comparable vertical effect during mandibular en-masse retraction with aligners and Class II elastics. The consistency of this division suggests that the type of elastic might be selected with reference to the vertical skeletal pattern: an intramaxillary elastic could be preferred where posterior intrusion is desirable, as in high-angle patients with an anterior open bite, whereas a Class II elastic might be considered where extrusion would assist in the reduction of a deep overbite.

The vertical crown–root difference requires careful interpretation. In the sagittal and transverse planes the crown landmarks and the apices are separated in a direction

perpendicular to the movement, so that their difference reflects rotation about a genuine moment arm. In the vertical plane they lie approximately on the same axis, and a rigid body can only produce differing vertical displacements at these landmarks if it rotates about an axis offset from them. Scenario 8 illustrates the consequence: the vertical crown–root difference was essentially zero, a value that considered alone might suggest bodily intrusion, yet the individual landmark values ranged from -0.076570 to $+0.006157\ \mu\text{m}$ (Table 3), which indicates that the near-zero difference arose from the coincidence of the crown and root means rather than from an absence of rotation. The choice of elastic may therefore determine the direction of vertical movement, but it does not appear to eliminate the accompanying rotational component.

The transverse findings suggest that the direction of buccolingual tipping is related to the vertical position at which the force is applied. Where force was delivered from a crown-level button, as in Scenarios 2, 3 and 4, the crown tipped lingually while the apices moved buccally, and the largest transverse crown–root difference of the series was recorded in Scenario 3 ($+1.093275\ \mu\text{m}$), approximately 2.6 times that of the next highest scenario. Reduced effectiveness of aligners in controlling molar torque has been reported clinically by Papadimitriou et al. [27], and Machado [21] noted that the flexibility of the thermoplastic shell reduces predictability during space closure. The pattern observed in these scenarios is compatible with those observations, since a buccally applied force combined with transverse deformation of the aligner would be expected to generate a lingual crown moment.

Where the force was transmitted through a lever arm to a maxillary miniscrew, as in Scenarios 5 and 6, the direction of transverse tipping reversed and buccal crown tipping was observed (-0.287045 and $-0.412750\ \mu\text{m}$), even though the type of elastic was the same as in Scenario 2. Since the only difference between these configurations was the presence of the lever arm, it may be inferred that moving the point of force application apically can invert the

transverse moment. The importance of the point of force application in torque expression with aligners was demonstrated experimentally for incisors by Hahn et al. [30], and the present results suggest that the same principle extends to the transverse behaviour of mandibular molars. In these two scenarios the apices moved approximately three times as far as the crown, so that the tooth as a body shifted lingually while the crown tipped buccally (net transverse displacement +0.067078 and +0.080925 μm). This combination of a large tipping component with a net transverse body shift might disturb posterior occlusal contacts, and it would seem advisable to weigh this against the extrusive benefit that these configurations may offer in deep bite cases.

Transverse control was most favourable in Scenario 7 (+0.053125 μm), Scenario 10 (+0.063095 μm) and Scenario 1 (+0.088370 μm). Within both elastic groups the lever arm angulated 30° distally was associated with the smallest transverse crown–root difference, which suggests that distal angulation may limit tipping in the transverse plane as well as in the sagittal plane.

Peak stress in the PDL was only moderately associated with the magnitude of movement ($p = 0.65$), and two scenarios departed from the general trend. Scenario 8 showed the fourth lowest total displacement yet the highest peak stress, which may be explained by the concentration of force in the apical region through the lever arm and the consequent localization of stress within a restricted area of the ligament. Scenario 3 showed the opposite pattern, the largest total displacement being accompanied by only the fourth highest peak stress, which suggests that stress was distributed over a wider area. Peak stress therefore appears to reflect the distribution of the force rather than the amount of movement, an observation that may be relevant to the risk of root resorption, which has been related to the character of the applied load [31, 32]. A similar caution regarding the interpretation of total displacement was expressed by Qiang et al. [29], who examined posterior anchorage loss under different

extraction patterns with clear aligners. Scenario 10 combined the lowest maximum and the lowest minimum stress with the lowest total displacement and the lowest sagittal tipping, and on the basis of these findings it is considered that this configuration may represent the most balanced force system among those examined.

Taken together, these findings indicate that the two design variables act predominantly on different planes. The type of elastic determines the vertical direction of movement, whereas the angulation of the lever arm governs the magnitude of tipping and, in the transverse plane, its direction. Clinically, this may allow the two decisions to be considered separately, the elastic being chosen with reference to the vertical skeletal pattern and overbite, and the lever arm angulation according to the degree of sagittal and transverse control required.

Limitations

Several limitations apply. The analysis is static and linear, and the tissues were assumed to be homogeneous and isotropic, so the viscoelastic behaviour of the PDL and time-dependent biological processes such as bone remodelling were not represented. Only a single 0.25 mm activation was simulated, and the results describe the initial elastic response rather than the cumulative movement achieved over a sequence of aligners.

Bonded contact was defined between the aligner and the tooth surfaces. This assumption excludes the slippage and loss of fit that occur clinically, and consequently the computed displacements represent an upper bound on what would be expected in the mouth.

Stress in the PDL was evaluated using the von Mises criterion, which is a scalar quantity and does not distinguish compression from tension. Since bone resorption and apposition depend on that distinction, the stress values should be read as a comparative index of total mechanical loading rather than as a direct predictor of tissue response.

Bone resorption and changes in bone density that follow the healing of an extraction socket were not modelled, although they may alter the biomechanics of molar mesialization in long-standing edentulous sites. Finally, movement was characterized from six landmarks; rotation about the long axis of the tooth was not quantified separately, and estimating it reliably would require a rigid-body fit to the three-dimensional coordinates of the landmarks. This remains a subject for further work.

Conclusions

Within the limitations of this finite element analysis, mesial tipping was the predominant response during mandibular molar mesialization with clear aligners, and the two design variables examined acted on different planes. The type of elastic determined the direction of vertical movement in all ten configurations, Class II intermaxillary elastics being associated with extrusion and intramaxillary elastics with intrusion. The angulation of the auxiliary lever arm governed the magnitude of sagittal tipping and, in the transverse plane, was able to reverse its direction.

A lever arm angulated 30° distally to the long axis of the tooth, combined with an intramaxillary elastic, produced the lowest tipping in all three planes, the lowest total displacement and the lowest periodontal ligament stress. On the basis of these findings it is considered that this configuration may represent the most biomechanically balanced of those examined. Clinical studies would be required to confirm these comparative trends.

List of abbreviations

CBCT: Cone-beam computed tomography

DBCT: Distobuccal cusp tip

DLCT: Distolingual cusp tip

DRA: Distal root apex

FEA: Finite element analysis

MBCT: Mesiobuccal cusp tip

MLCT: Mesiolingual cusp tip

MM2: Mandibular second molar

MRA: Mesial root apex

PDL: Periodontal ligament

Declarations

Ethics approval and consent to participate

The study was approved by the Hamidiye Scientific Research Ethics Committee of the University of Health Sciences, Istanbul, Türkiye (approval number 24/584, dated 20 September 2024). The study was performed in accordance with the Declaration of Helsinki. The finite element models were derived from an anonymized archival cone-beam computed tomography data set; the requirement for individual informed consent was waived by the same ethics committee.

Consent for publication

Not applicable.

Availability of data and materials

All data generated or analysed during this study are included in this published article. The finite element models are available from the corresponding author on reasonable request.

Competing interests

The authors declare that they have no competing interests.

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Authors' contributions

EC and ŞK conceived and designed the study. EC constructed the finite element models, performed the analyses and prepared the tables and figures. ŞK supervised the work and validated the biomechanical interpretation. EC drafted the manuscript and ŞK revised it critically for important intellectual content. Both authors read and approved the final manuscript.

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Authors' information

Not applicable.

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Figure legends

Fig. 1 Displacement of the mandibular second molar along the X-axis

Contour plots of sagittal displacement for the ten scenarios. Warm colours indicate greater displacement magnitude. Each panel shows the mandibular second molar with the corresponding scale bar and coordinate triad.

Fig. 2 Sagittal displacement components of the mandibular second molar

a Net sagittal displacement, representing the translational component, calculated as the mean of crown and root displacement. b Crown–root difference along the X-axis, representing the rotational component. Negative values indicate mesial direction in a and mesial tipping in b.

Fig. 3 Displacement of the mandibular second molar along the Y-axis

Contour plots of vertical displacement for the ten scenarios. Warm colours indicate greater displacement magnitude. Each panel shows the mandibular second molar with the corresponding scale bar and coordinate triad.

Fig. 4 Vertical displacement components of the mandibular second molar

a Net vertical displacement, representing the translational component; negative values indicate intrusion and positive values extrusion. b Crown–root difference along the Y-axis. As explained in the Methods, this quantity reflects the vertical projection of buccolingual tipping and is not a measure of intrusion or extrusion.

Fig. 5 Displacement of the mandibular second molar along the Z-axis

Contour plots of transverse displacement for the ten scenarios. Warm colours indicate greater displacement magnitude. Each panel shows the mandibular second molar with the corresponding scale bar and coordinate triad.

Fig. 6 Transverse displacement components of the mandibular second molar

a Net transverse displacement, representing the translational component; positive values indicate lingual direction. b Crown–root difference along the Z-axis; positive values indicate lingual crown tipping and negative values buccal crown tipping.

Fig. 7 Von Mises stress distribution in the periodontal ligament

Contour plots of von Mises stress in the periodontal ligament of the mandibular second molar for the ten scenarios. Warm colours indicate higher stress. Each panel shows the corresponding scale bar.

Fig. 8 Von Mises stress in the periodontal ligament by scenario

a Maximum von Mises stress. b Minimum von Mises stress. Values are expressed in kilopascals.

Fig. 9 Relationship between vertical and transverse crown–root differences

Scatter plot of the vertical crown–root difference against the transverse crown–root difference for the ten scenarios; numbers identify the scenario. The dashed line is the least-squares fit through the origin. The signs of the two quantities are opposite in every scenario, indicating that the vertical crown–root difference reflects buccolingual rather than vertical rotation.

Tables

Table 1 Scenario definitions with node and element counts of the finite element models

Scenario	Configuration	Nodes	Elements
Scenario 1	Aligner only	81399	358561
Scenario 2	Buccal button + Class II elastic	97289	437468
Scenario 3	Buccal button + intramaxillary elastic	97289	437468
Scenario 4	Mesiolingual button + Class II elastic	81627	363006
Scenario 5	Buccal lever arm 0° + Class II elastic	95104	427700

Scenario	Configuration	Nodes	Elements
Scenario 6	Buccal lever arm 30° mesial + Class II elastic	95265	427989
Scenario 7	Buccal lever arm 30° distal + Class II elastic	95043	426804
Scenario 8	Buccal lever arm 0° + intramaxillary elastic	102612	454482
Scenario 9	Buccal lever arm 30° mesial + intramaxillary elastic	102773	454771
Scenario 10	Buccal lever arm 30° distal + intramaxillary elastic	102597	453738

Each scenario was modelled separately; mesh density varied with the auxiliary elements included in the model.

Table 2 Material properties assigned to the finite element models

Material	Young's modulus (MPa)	Poisson's ratio
Compact bone	13000.00	0.30
Cancellous bone	1370.00	0.30
Tooth	18600.00	0.31
Periodontal ligament	0.68	0.45
Stainless steel (button and lever arm)	210000.00	0.30
Miniscrew (titanium alloy)	113763.35	0.35
Clear aligner	528.00	0.36
Attachment	12500.00	0.36

All materials were assumed to be linear, homogeneous and isotropic. Values were taken from published data [2].

Table 3 Displacement of the six landmarks of the mandibular second molar along the three axes

Scenario	Landmark	X-axis (µm)	Y-axis (µm)	Z-axis (µm)	Total (µm)
Scenario 1	MBCT	-0.012490	-0.033650	+0.056370	0.06683
	MLCT	-0.008925	-0.024710	+0.041560	0.04917
	DBCT	-0.004000	-0.002796	+0.048400	0.04865
	DLCT	-0.002370	+0.002164	+0.044310	0.04443
	MRA	+0.004071	-0.003297	-0.044000	0.04431
	DRA	+0.006261	+0.012050	-0.037420	0.03981
Scenario 2	MBCT	-0.123600	-0.056280	+0.141500	0.19613
	MLCT	-0.090330	-0.061430	+0.078210	0.13435
	DBCT	-0.076390	+0.015200	+0.154800	0.17329
	DLCT	-0.052610	+0.003189	+0.095020	0.10866
	MRA	+0.065620	+0.023400	-0.106000	0.12684
	DRA	+0.079609	+0.069030	-0.085440	0.13566
Scenario 3	MBCT	-0.033010	-0.390600	+0.533200	0.66179
	MLCT	-0.020410	-0.267800	+0.402600	0.48396
	DBCT	+0.004922	-0.079280	+0.577900	0.58333
	DLCT	+0.001592	+0.056280	+0.432000	0.43565
	MRA	+0.002414	-0.042980	-0.629300	0.63077
	DRA	+0.016840	+0.128500	-0.584400	0.59860
Scenario 4	MBCT	-0.009947	-0.047740	+0.111100	0.12133
	MLCT	-0.014270	-0.028780	+0.110600	0.11517
	DBCT	-0.028460	+0.011610	+0.116100	0.12010
	DLCT	-0.031510	+0.021430	+0.116500	0.12257
	MRA	-0.012080	+0.014540	-0.106900	0.10856
	DRA	-0.016960	+0.048250	-0.105500	0.11724
Scenario 5	MBCT	-0.117500	+0.133700	-0.062210	0.18855
	MLCT	-0.077770	+0.066250	-0.084660	0.13268
	DBCT	-0.056890	+0.051930	-0.070320	0.10430
	DLCT	-0.037250	+0.010070	-0.088590	0.09663
	MRA	+0.070020	+0.049560	+0.207800	0.22481

Scenario	Landmark	X-axis (µm)	Y-axis (µm)	Z-axis (µm)	Total (µm)
Scenario 6	DRA	+0.079840	+0.011700	+0.213400	0.22815
	MBCT	-0.131500	+0.162300	-0.114800	0.23835
	MLCT	-0.089740	+0.091530	-0.132200	0.18414
	DBCT	-0.058740	+0.056220	-0.117800	0.14314
	DLCT	-0.037610	+0.008181	-0.137000	0.14230
Scenario 7	MRA	+0.058270	+0.055030	+0.286000	0.29702
	DRA	+0.073230	-0.007103	+0.288600	0.29783
	MBCT	-0.016780	-0.006432	+0.035400	0.03970
	MLCT	-0.013400	-0.007230	+0.028080	0.03194
	DBCT	-0.014790	+0.010180	+0.037610	0.04168
Scenario 8	DLCT	-0.011810	+0.007461	+0.030750	0.03377
	MRA	+0.016270	+0.012240	-0.021320	0.02948
	DRA	+0.017300	+0.022570	-0.019010	0.03421
	MBCT	-0.009346	-0.076570	+0.083510	0.11368
	MLCT	-0.015850	-0.031170	+0.019690	0.04013
Scenario 9	DBCT	+0.041830	-0.050380	+0.098830	0.11855
	DLCT	+0.042840	+0.006157	+0.027280	0.05116
	MRA	-0.108000	-0.043930	-0.067300	0.13462
	DRA	-0.078310	-0.029920	-0.048770	0.09699
	MBCT	-0.054230	-0.111700	+0.158600	0.20142
Scenario 10	MLCT	-0.052500	-0.072570	+0.065940	0.11122
	DBCT	+0.009313	-0.047980	+0.177600	0.18420
	DLCT	+0.016620	-0.001483	+0.091790	0.09329
	MRA	-0.081580	-0.036580	-0.158600	0.18206
	DRA	-0.046600	+0.005341	-0.131400	0.13952

MBCT mesiobuccal cusp tip, MLCT mesiolingual cusp tip, DBCT distobuccal cusp tip, DLCT distolingual cusp tip, MRA mesial root apex, DRA distal root apex. On the X-axis negative values indicate mesial and positive values distal displacement; on the Y-axis negative values indicate intrusion and positive values extrusion; on the Z-axis positive values indicate lingual and negative values buccal displacement. Total displacement is the vector magnitude of the three components.

Table 4 Sagittal displacement components of the mandibular second molar

Scenario	Crown (µm)	Root (µm)	Net (µm)	ΔX
Scenario 1	-0.006946	+0.005166	-0.000890	-0.012112
Scenario 2	-0.085733	+0.072614	-0.006559	-0.158347
Scenario 3	-0.011726	+0.009627	-0.001050	-0.021353
Scenario 4	-0.021047	-0.014520	-0.017783	-0.006527
Scenario 5	-0.072353	+0.074930	+0.001289	-0.147282
Scenario 6	-0.079397	+0.065750	-0.006824	-0.145147
Scenario 7	-0.014195	+0.016785	+0.001295	-0.030980
Scenario 8	+0.014868	-0.093155	-0.039143	+0.108023
Scenario 9	-0.020199	-0.064090	-0.042145	+0.043891
Scenario 10	-0.012299	-0.010506	-0.011402	-0.001793

Crown is the mean displacement of the four cusp tips and root the mean displacement of the two apices. Net is the mean of crown and root and represents translation; ΔX is crown minus root and represents rotation. Negative ΔX indicates mesial tipping and positive ΔX distal tipping.

Table 5 Vertical displacement components of the mandibular second molar

Scenario	Crown (μm)	Root (μm)	Net (μm)	Direction	ΔY
Scenario 1	-0.014748	+0.004377	-0.005186	Intrusion	-0.019124
Scenario 2	-0.024830	+0.046215	+0.010692	Extrusion	-0.071045
Scenario 3	-0.170350	+0.042760	-0.063795	Intrusion	-0.213110
Scenario 4	-0.010870	+0.031395	+0.010263	Extrusion	-0.042265
Scenario 5	+0.065488	+0.030630	+0.048059	Extrusion	+0.034857
Scenario 6	+0.079558	+0.023964	+0.051761	Extrusion	+0.055594
Scenario 7	+0.000995	+0.017405	+0.009200	Extrusion	-0.016410
Scenario 8	-0.037991	-0.036925	-0.037458	Intrusion	-0.001066
Scenario 9	-0.058433	-0.015620	-0.037026	Intrusion	-0.042814
Scenario 10	-0.013778	-0.002387	-0.008083	Intrusion	-0.011390

Net vertical displacement determines the direction of movement: negative values indicate intrusion and positive values extrusion. ΔY reflects the vertical projection of buccolingual tipping and is not a measure of intrusion or extrusion.

Table 6 Transverse displacement components of the mandibular second molar

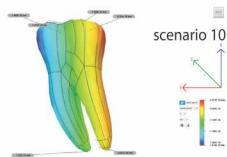
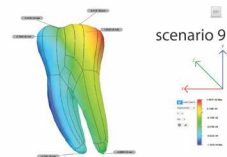
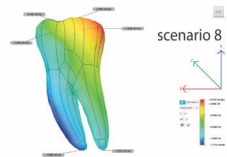
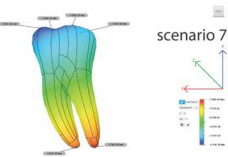
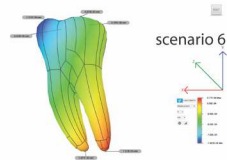
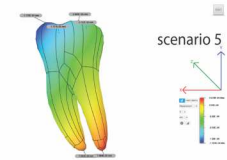
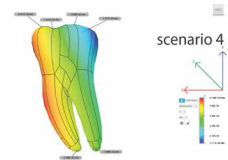
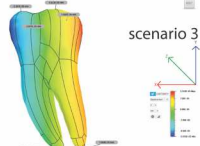
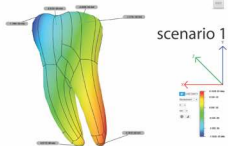
Scenario	Crown (μm)	Root (μm)	Net (μm)	ΔZ	Tipping direction
Scenario 1	+0.047660	-0.040710	+0.003475	+0.088370	Lingual crown tipping
Scenario 2	+0.117383	-0.095720	+0.010831	+0.213103	Lingual crown tipping
Scenario 3	+0.486425	-0.606850	-0.060213	+1.093275	Lingual crown tipping
Scenario 4	+0.113575	-0.106200	+0.003688	+0.219775	Lingual crown tipping
Scenario 5	-0.076445	+0.210600	+0.067078	-0.287045	Buccal crown tipping
Scenario 6	-0.125450	+0.287300	+0.080925	-0.412750	Buccal crown tipping
Scenario 7	+0.032960	-0.020165	+0.006398	+0.053125	Lingual crown tipping
Scenario 8	+0.057328	-0.058035	-0.000354	+0.115363	Lingual crown tipping
Scenario 9	+0.123482	-0.145000	-0.010759	+0.268482	Lingual crown tipping
Scenario 10	+0.019850	-0.043245	-0.011698	+0.063095	Lingual crown tipping

Net transverse displacement represents translation; positive values indicate lingual and negative values buccal direction. ΔZ represents rotation: positive values indicate lingual crown tipping and negative values buccal crown tipping.

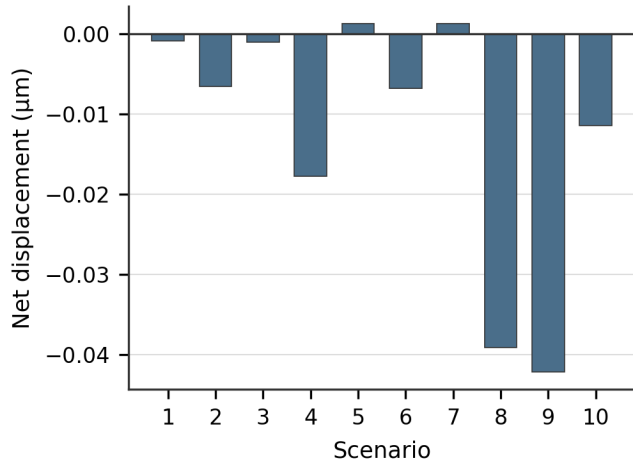
Table 7 Mean total displacement and von Mises stress in the periodontal ligament

Scenario	Mean total displacement (μm)	Maximum von Mises stress (kPa)	Minimum von Mises stress (kPa)
Scenario 1	0.04886	1.0000	0.001812
Scenario 2	0.14582	3.0000	0.002243
Scenario 3	0.56568	6.0000	0.010870
Scenario 4	0.11750	3.0000	0.003599
Scenario 5	0.16252	6.0000	0.003123
Scenario 6	0.21713	8.0000	0.004532
Scenario 7	0.03513	0.9109	0.000903
Scenario 8	0.09252	8.3032	0.002036
Scenario 9	0.15195	7.0836	0.001249
Scenario 10	0.03386	0.4643	0.000689

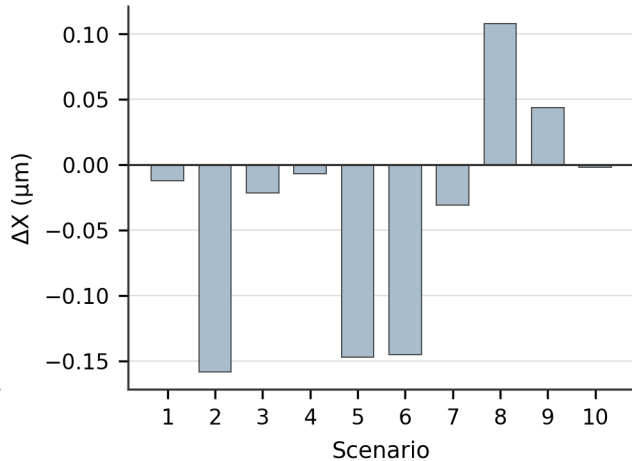
Mean total displacement is the arithmetic mean of the total displacement of the six landmarks. Stress values were converted from the solver output expressed in MPa.

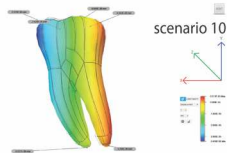
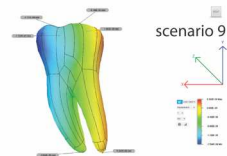
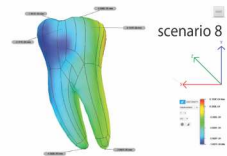
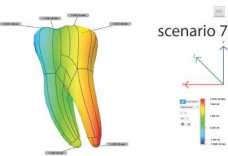
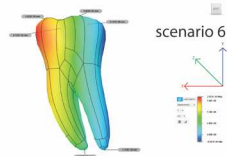
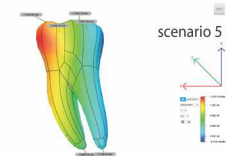
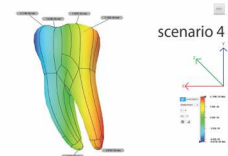
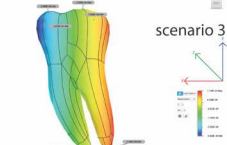
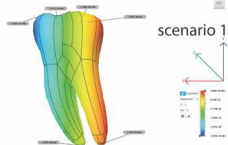


a Net mesiodistal displacement

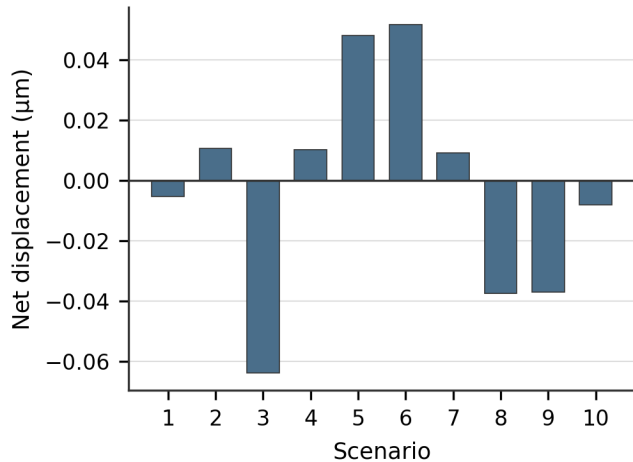


b Crown-root difference (tipping)

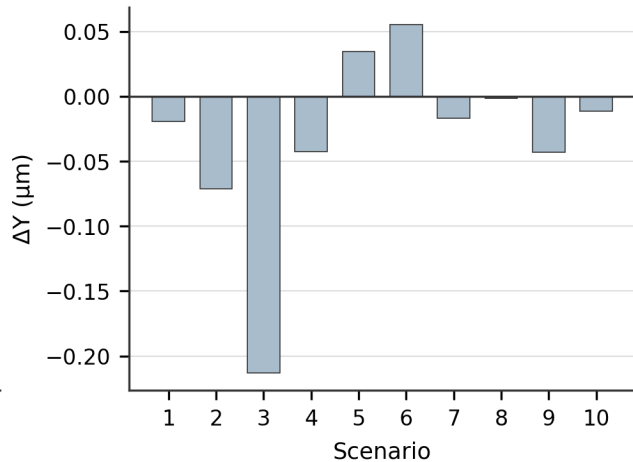


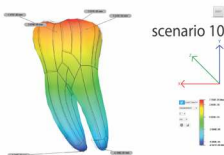
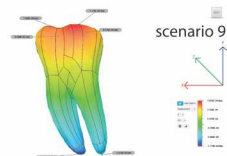
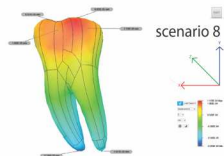
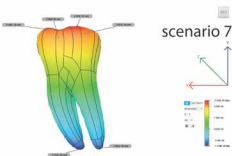
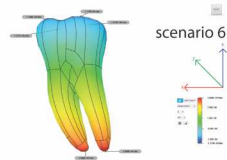
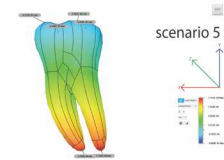
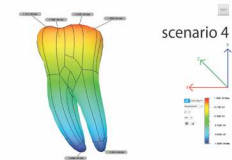
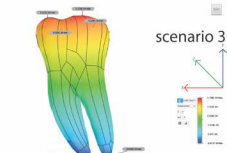
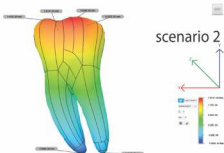
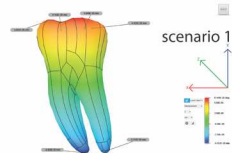


a Net vertical displacement

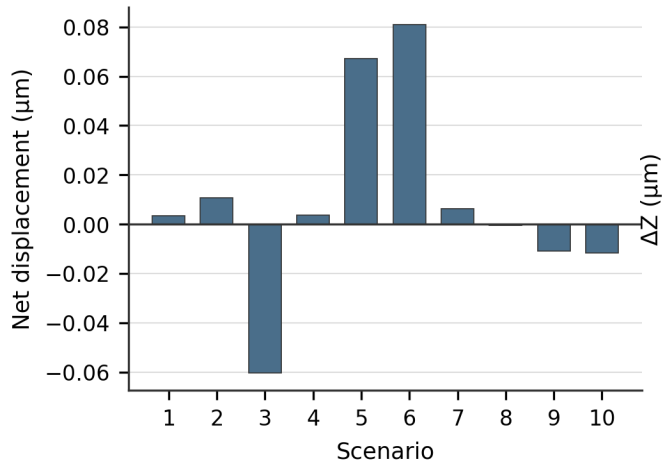


b Crown-root difference

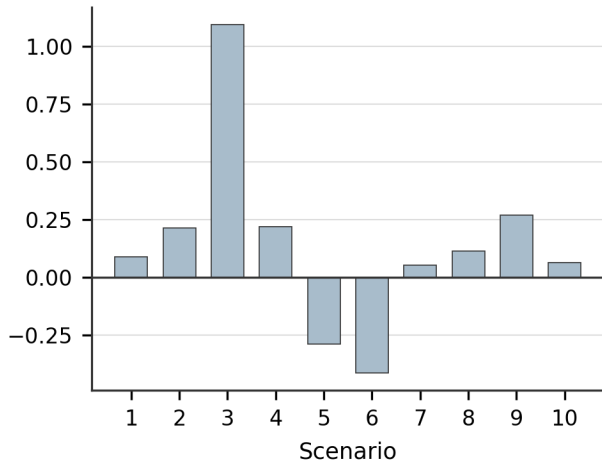


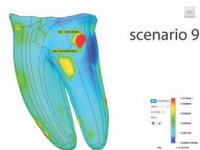
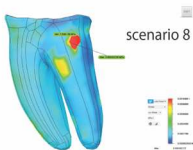
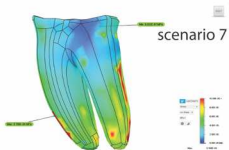
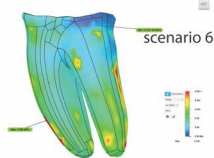
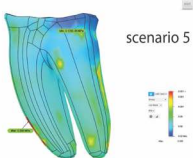
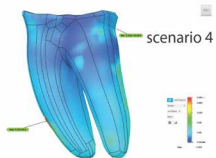
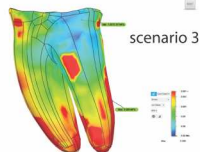
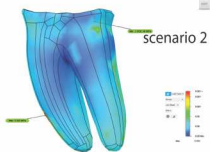
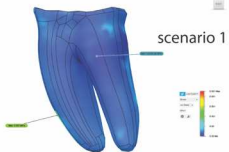


a Net transverse displacement

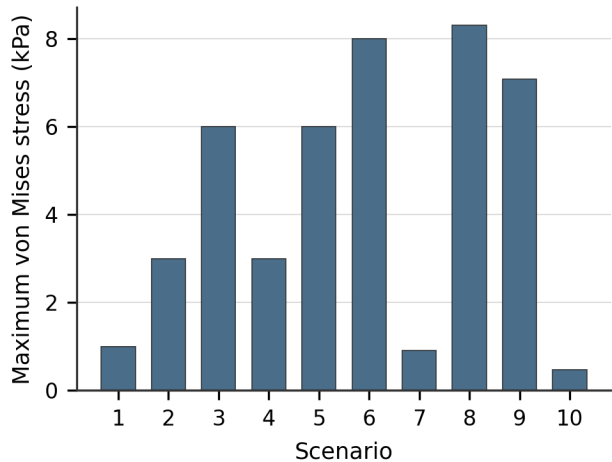


b Crown-root difference (tipping)

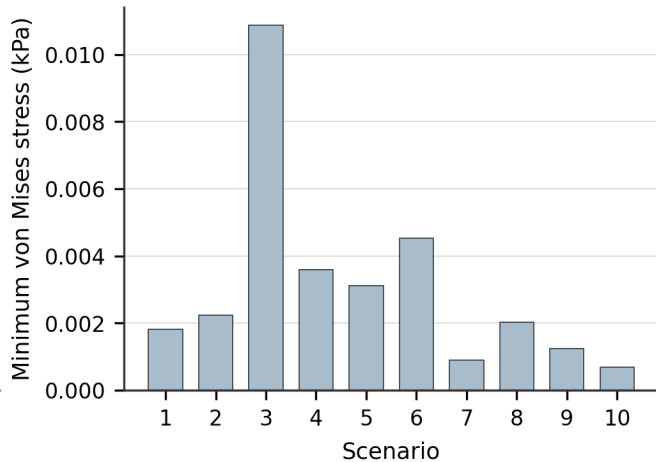




a Maximum von Mises stress



b Minimum von Mises stress



ΔY , vertical crown-root difference (μm)

--- $r = -0.98$

