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RESEARCH PAPER

Investigation of the Behavior of Different Ni-Ti Dental Files and Chemical Mechanical Behavior Using Finite Element Analysis

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ABSTRACT

Rotary files with superelastic qualities have received attention in dentistry field with gold standard for endodontic procedures such as root canal preparation and shaping. Despite their high flexibility, files within root canals can fracture. The most common causes of file fractures are bending and torsional forces. Therefore, manufacturers attempt to enhance the mechanical properties in order to resist such forces and pressures. Many factors, including the instrument-making process, alloy's characteristics, as well as file geometry and features like pitch length and taper may impact the mechanical performance of the files. The aim of the present study was to investigate the effect of file geometry on file resistance to flexural and torsional stresses. This work was conducted as an experimental analysis using finite element analysis (FEA). The NiTi file was characterized using X-ray diffraction (XRD) analysis. Four different endodontic files including Vortex Blue, Edge File, One Curve and Hyflex-EDM with the same tip and diameter, and different geometric features were designed using SolidWorks software. These models were then transferred to ANSYS, a three-dimensional (3D) modeling program, and examined under torsional and flexural forces. In order to simulate rotational stress, the file shank was fixed and rotated at $\theta = 22°$. In additon, a 3.8 mm file was bent on the Y axis for simulating flexural stresses. The Edge File and Vortex Blue file had the highest and lowest amounts of flexural and torsional stress, respectively. Further, in all the samples the highest amount of torsional stress was observed at 2 to 3 mm of the file tip while the highest amount of flexural stress was seen in the depth of the flutes and near the winning edges. The four examined endodontic instruments had different mechanical properties due to their different geometry. For a good and longer-lasting root canal treatment, dentists should utilize an appropriate file based on manufacturing instructions and clinical conditions.

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INTRODUCTION

Aluminum-titanium alloys are known for their low elastic modulus and distinct quasi-elastic properties. Because of their mechanical characteristics, they are an ideal choice for manufacturing endodontic files [1]. Nickel-titanium (NiTi) rotary files are 2 to 3 times more flexible than stainless steel (SS) files and, in particular, have better angular deviations and maximum torque to failure [2-4]. For many years, these files have been utilized for improving the effectiveness and speed of curing even in highly curved channels. Titanium alloys are highly recommended due to their superelasticity [5-8]. Sattapan et al. [9] evaluated a canal filling with some errors such as elongation, canal transport, and perforations. One of the most common mistakes is file breakage and sudden fracture. File fractures of manual files and rotary files occur in 1 to 6% and 0.4 to 5% of cases,

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respectively. Evaluation of mechanical properties of endodontic files can improve clinical application and minimize their fractures and channel blockage. Because of the flexibility of NiTi tools, NiTi files may undergo significant deformation while retaining their original shape within their superelastic range [10-14]. The flexibility of NiTi instruments is vital in the effective treatment of endodontics, especially in curved canals which promotes proper canal enlargement while maintaining the instrument in a central position within the canal and minimizing undesirable changes in the form of curved canals [15-18]. The new generation of NiTi endodontic files with enhanced mechanical properties has been developed through a series of mechanical heat treatments such as producing NiTi alloys with martensite phase [19-22].

Various alloys are malleable in the form of martensite as a wire; they deform readily and become more flexible than austenite. Thus, reducing the risk of fracture under high stress is more commen [23-29]. However, no material is safe to fracture and may break as the pressure exceeds its ultimate strength [30-36]. Nitinol alloy is one of the most intriguing smart materials applied in bone surgery and making artificial muscles. The biocompatibility of this material is of great importance depending on the type of application [37-41]. Due to its special and potential properties, this new material has been used in engineering applications such as robotic actuators, memory composites, and medical implants. The casting method presents a significant challenge in producing nitinol alloys with precise chemical composition and without deleterious contamination. Powder metallurgy has drawn researchers' attention as a viable method for making and producing nitinol alloys [42-45]. It should be noted that no manual or rotary files are ideal for all clinical cases [46-51]. Due to its ultra-elastic mechanical properties, NiTi rotary files have become the best choice for cleaning and shaping the roots. The ultra-elastic properties increase the flexibility and enable the instruments to effectively follow the main path of the channel [46-52]. However, during canal preparation, endodontic files are subjected to torsional and flexural forces due to the friction between the file and the tooth wall and the canal-curved path. Excessive friction of the root canal path increases the risk of breaking the tip of the file in the canal and blocking the canal path, which is especially concerning for small files. Alfouzan et al. [16] reported that a higher percentage of deformation occurs in small files. Some authors have attributed file failure to fatigue caused by repeated bending stresses in curved channels, while others have blamed the twisting force on the file failure. Twisting occurs as the file is locked against a canal wall or when a clinician applies force to the file. Regardless of the cause of these failures, the treatment's result may be compromised. Despite the fact that these two elements are considered separately, torsional fatigue and bending must be analyzed jointly [53-58]. Cyclic prestressing can reduce the torsional strength of files. Bending leads to the highest surface stress near the winning edge, whereas torsional force cuases the highest stress concentration towards the end of the flute in U-shaped designs. In this work, the mechanical stress of various types of files was investigated using finite element analysis.

MATERIALS AND METHOD

Based on earlier research, the design of the cross section and the number of file threads have a major effect in the mechanical behavior of rotary files under torsional and flexural stresses. According to the study, there is no specific sample size and measurement method; therefore, this simulation was performed using various specifications to establish the exact form and mathematical simulation for predicting the nature of file failure. The FEA describes a physical model and divides it into smaller elements in order to prepare a mesh model. Since each element of the form has its own structure and material properties, the interrelationships between the elements called nodes can be routinely investigated using various computer algorithms. The FEA is a reproducible analysis method which was performed in a computer environment. The FEA examines stress and deformation and solves complex structural problems. Accordingly, the FEA may be a reliable tool for evaluating the behavior of NiTi rotary files, allowing different tool designs to be tested under different loading conditions, thus saving tool time and expense. The aim is to observe various metallurgical effects between different types of NiTi or other alloys and to identify the forces generated during the formation of the root canal. In this study, the cross-sectional design was the main parameter examined in terms of geometric variances. In addition, the mechanical properties of four types of endodontic files including HyFlex EDM (Coltene), Vortex Blue (DEntsply), OneCurve (Micro Mega), and Edge File X3 (Edge Endo) under bending and torsional forces were investigated. HyFlex EDM (Coltène/Whaledent Inc., Altstäten, Switzerland) is a single-file system that was used as a continuous rotation. These files are made by electrically discharged machining (EDM) of controlled memory (CM) wire since non-contact spark abrasion is used to shape the files, thus eliminating the stress of traditional methods [20-23]. This file's cross section is variable, and the third part is coronal, in the shape of a triangle; the middle third of the file is trapezoidal, and the third part is apical, in the shape of a rectangle. Further, the EdgeFile X3 (EFX3; EdgeEndo, New Mexico, USA), which is made by fire-wire heat treatment from a controlled memory (CM) wire, has a cross-sectional surface modified into a convex triangle. This system has seven files including an orifice opener NX (25,12), two files to enlarge the coronal part of the crown N1 (17,04) and N2 (17,06), and four files to complete the apical part C1 (20,06), C2 (25.06), C3 (30.06) and C4 (40.06(3.

Vortex Blue (Dentsply Tulsa Dental Specialties, Tulsa, OK, USA) is made from an alloy that undergoes a complex heating and cooling operation which gives the alloy a blue color with a visible titanium oxide layer on the coated surface. These systems contain more stable martensite than M wire, increasing the softness and ductility of the alloy [24-29]. The cross-section of this file is a convex triangle. This system has been introduced to the market from file number 15 to 50 with duplicators 0.04 and 0.06. Another type of files is One Curve (Micro Mega, Besançon, France) which is a single file system made of heat-treated C-Wire. For improved focusing and dentin cutting efficiency, the system also has a variable cross-section in the form of an S-Shape in the coronal section and an asymmetrical convex triangle in the apical part. According to the manufacturer, this device has a controlled memory, which allows it to bend prematurely, increasing the formation of the root canal.

Reconstruction of 3D model

Various methods are used to help modeling the geometry of files. Arbab-Chirani et al. studied and were able to produce endodontic files numerically from the catalogs and specifications published by the manufacturer [3]. Using reverse engineering process a duplicate is produced which is substantially comparable to a real endodontic file [59-64]. In the current study, the catalogs published by the company were utilized to obtain the geometry of the files, and the files were also inspected using a light microscope for further detail. Then, a 3D models of these four endodontic files including Vortex Blue (Dentsply), Edge file (Edge Endo), Hyflex EDM (Coltene), and One Curve (Micro Mega) with the same diameter of 0.25mm, convergence of 0.06- and 25-mm file length, and having different cross-sectional shapes was designed by Computer-Assisted Design (CAD) software and developed by SOLIDWORKS® 2021

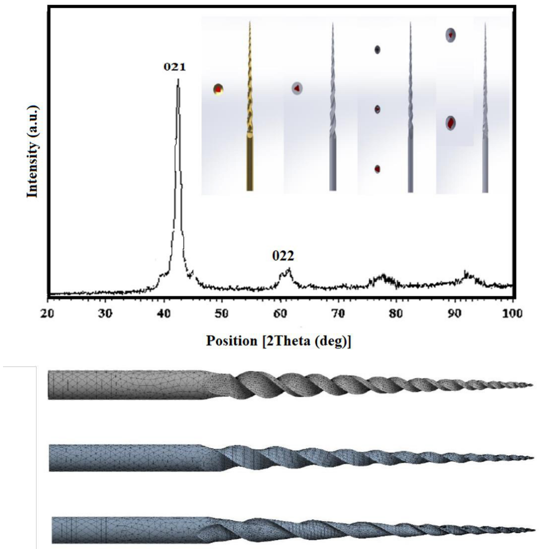

Fig. 1. XRD pattern and design of files including Vortex Blue (32564elements), Edge File (15610elements), Hyflex EDM (19046elements), and One Curve (22488elements) and modeling of models.

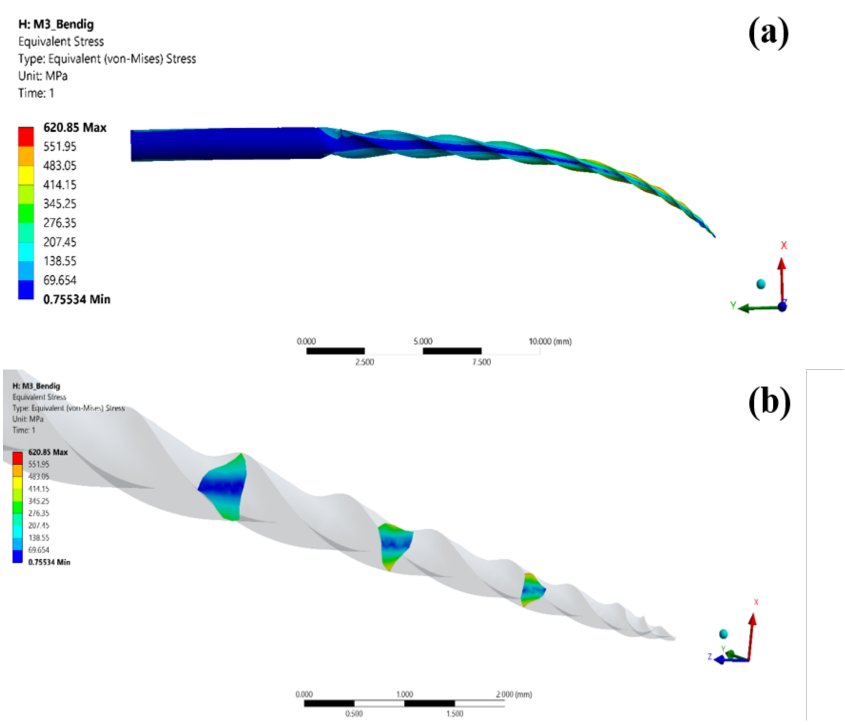

Fig. 2. Bending stresses of a) Edge Endo file (longitudinal view of the file), and b) torsion stresses in the Edge Endo file (transverse view of the file).

(Dassault Systèmes, SolidWorks Corp., Concord, MA, US).

RESULTS AND DISSCUSION

Fig. 1 depicts the design of files, from right to left: Vortex Blue, Edge File, Hyflex EDM, and One Curve. Endodontic rotary files are usually composed of NiTi or Nitinol-Titanium alloy (Naval Ordinance factory) and manifest highly non-linear behavior as seen in Fig. 1 and Fig. 2. The first part of the stress-strain curve is linear, and the alloy is in the more stable crystalline phase, the austenitic phase. The second part of the stress-strain curve is likewise linear but nearly flat, indicating a transition phase in which each little stress exerts a significant amount of pressure. Fig. 1 demonstrates the X-ray diffraction pattern of NiTi in which most sharp peaks occurred at 45-60°.

Fig. 2 indicates the bending stresses of the longitudinal view of the file as well as torsion stresses in the transverse view of the file. It demonstrates the super-elastic behavior of NiTi materials. The graph is very nonlinear with martensitic phase in the third phase of the stress-strain curve, indicating the typical stress-strain relationship for the fracture point metal. The observation shows that raising the stress gradually increases the strain. It should be mentioned that NiTi is particularly flexible and can withstand greater pressures that aid in cleaning and forming the root canal system. The considered elastic modulus in this study is about 36,000 MPa and the Poisson ratio of 0.3 is considered in the FEM analysis of these files as shown in Table 1 [42-45].

After designing the files, the geometry of the models is transferred to ANSYS®2021 finite element analysis software (Canonsburg, Pennsylvania, U.S) and the mechanical properties of the models including elastic modulus and Poisson's coefficient are defined. The meshing of the files and the number of elements is shown in Fig. 3. In order to exert force, most researchers have used the conditions mentioned in ISO 3630-1 International Specifications [14, 19]. In the present study, the amount of force entered by Arbab-Chirani et al. was applied [3].

These load values are selected to highlight the phase shift and to illustrate the superelastic properties of endodontic files. These models are then placed in boundary condition. For applying the bending forces, the file is fixed from the shank and the tip of the file bends by 3.8 mm as shown in Fig. 3. The mechanical behavior of NiTi files is assessed against flexural and torsional stresses

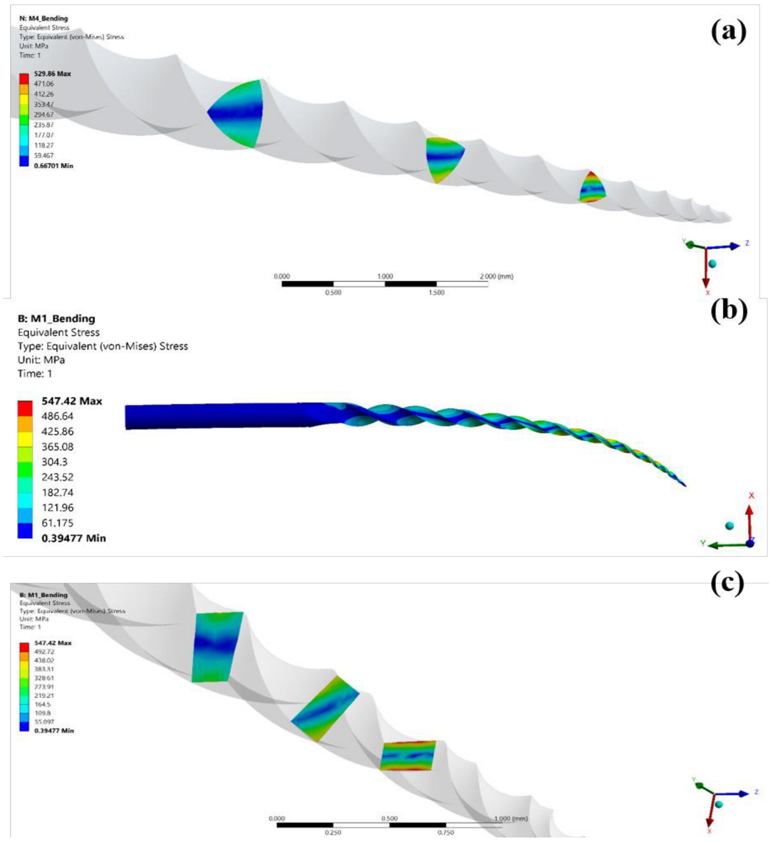

Fig. 3. a) Bending stresses distributed in the Edge Endo file (longitudinal view of the file), b) distributed torsion stresses in the Edge Endo file (transverse view of the file) and c) in Vortex blue file (transverse view of the file).

under the impact of various factors including the alloy's inherent properties as well as the design and engineering of the files. In this study, we investigated the effect of file geometry on how stress is distributed in the files. The following diagrams may show how stress is distributed in files against the exertion of flexural and torsional forces. The minimum and maximum values of stress are shown in blue and red, respectively. Based on Fig. 3, the maximum amount of stress, which was observed in the winning edges, is 547.42 MPa due to bending the tip of the Hyflex EDM file by 3.8 mm. According to the stress-strain diagram of NiTi alloy and the stress distribution in the file, it can be claimed that the file was subjected to the forces applied in the phase transition, i.e the conversion of the austenite phase to martensite.

The amounts of flexural forces increase towards the tip of the file (Fig. 3). Further, the amounts of forces from the center to the outer walls of the file are increased so that the maximum amounts of flexural forces enter the depth of the flutes. As shown in Fig. 3, due to the rotation of the tip of the Hyflex EDM file to 22°, the maximum amount of

Table 1. Von Mises stress levels of NiTi.

Sample	Maximum	Misses stress (MPa)
	Bending	Torsion
Hyflex EDM	547.42	570.35
One curve	534.8	561.56
Edge File	620.85	573.6
Vortex blue	529.86	544.37

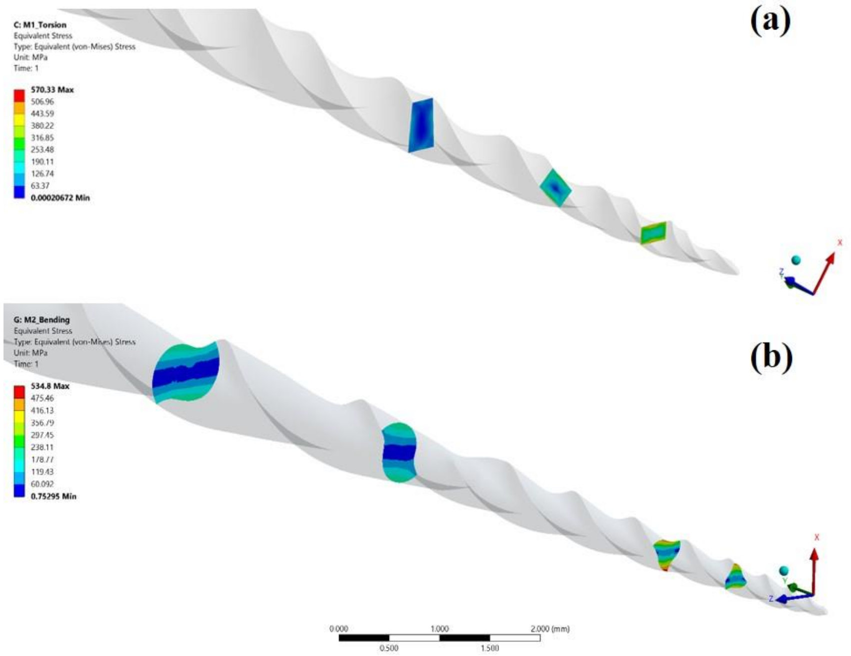

Fig. 4. a) Torsion stress is distributed in Hyflex EDM file (transverse view of the file) and b) distribute the stresses caused by bending in the One Curve file (transverse view of the file).

stress was reported to be 570.33 MPa. Furthermore, the highest amount of stress was observed near the top of the file. According to the stress-strain diagram of NiTi alloy and the stress distribution in the file, it can be claimed that the file was under the forces applied in the phase transition, i.e the conversion of the austenite phase to martenite.

According to Fig. 4 (a-c), the maximum amount of stress, observed in the winning edges, was reported as 534.8 MPa due to bending the tip of the One Curve file by 3.8 mm. Based on the stress-strain diagram of NiTi alloy and the stress distribution in the file, it can be claimed that the file was under the forces applied during the phase transition, i.e the conversion of the austenite phase to martensite. As shown in Fig. 4, the amounts of bending forces increase towards the tip of the file. Moreover, the amounts of forces from the center towards the outer walls of the file are increased so that the maximum amounts of bending forces enter the depth of the flutes.

Based on Fig. 4, the maximum amount of stress, observed near the top of the file, was reported as 561.57 MPa due to the rotation of the tip of the One Curve file to 22°. According to the stress-strain diagram of NiTi alloy and the stress distribution in the file, it may be concluded that the file was subjected to the forces applied in the transition phase, i.e the conversion of the austenite phase to martenite. According to Fig. 4, the amounts of torsional forces increase towards the top of the file. Further, the amounts of forces from the center to the outer walls of the file are increased so that the maximum amounts of torsional forces enter the depth of the flutes.

The maximum amount of stress, observed in the winning edges, was reported to be 620.85 MPa due to bending the tip of the Edge Endo file by 3.8 mm (Fig. 4). According to the stress-strain diagram of NiTi alloy and the stress distribution in the file, it is possible to conclude that the file was under the forces applied in the phase transition, i.e the conversion of austenite to martensite. According to Fig. 5, the amounts of bending forces increase towards the top of the file. Moreover, the amounts of forces from the center to the outer walls of the file are increased so that the maximum amounts of flexural forces enter the depth of the flutes.

Fig. 5 (c) shows that the maximum amount of stress applied is 573.6 MPa due to the rotation of the Edge Endo file tip to 22°. Further, the highest amount of stress was observed near the top of the file. According to the stress-strain diagram of NiTi alloy and the stress distribution in the file, it can be claimed that the file was under the forces applied in the transition phase, i.e the conversion of the

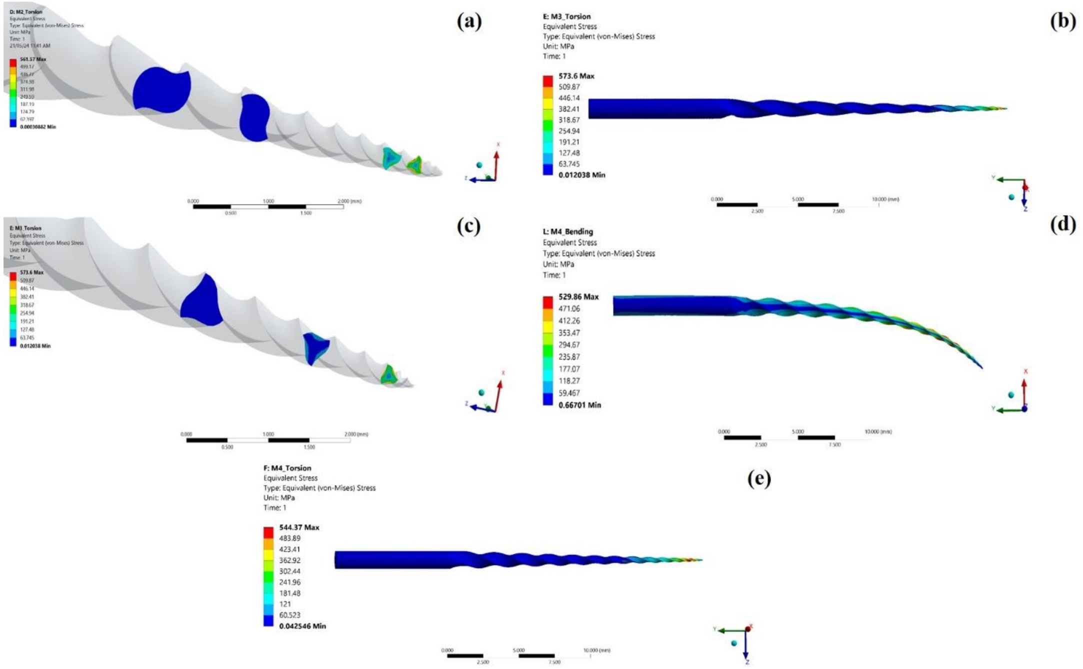

Fig. 5. Torsion distributes stresses a) in the one curve file (transverse view of the file), b) in the Edge Endo file (longitudinal view of the file), c) in the Edge Endo file (longitudinal view of the file), d) bending stresses in Vortex blue file (longitudinal view of the file) and e) distribute torsion stresses in the Vortex blue file (File length view).

austenite phase to martenite. As shown in Fig. 5, the amounts of torsional forces increase towards the top of the file. Furthermore, the amounts of force from the center towards the outer walls of the file are increased so that the maximum amounts of torsional forces enter the depth of the flutes. Based on Fig. 6, the highest amount of stress, observed in the winning edges, was reported to be 529.86 MPa due to bending the tip of the Vortex blue file by 3.8 mm. According to the stress-strain diagram of NiTi alloy and the stress distribution in the file, it is reasonable to assume that the file was under the forces applied in the phase transition, i.e the phase conversion of austenite to martensite.

According to Fig. 6, the amounts of bending forces increase tpwards the top of the file. In addition, the quantities of force applied from the center the file's outer walls are raised such that the maximum amounts of bending forces penetrate the depth of the flutes. The highest amount of stress, observed near the top of the file, was reported as 544.37 MPa due to the rotation of the tip of the Vortex blue file to 22° (Fig. 6). By investigating the stress-strain diagram of NiTi alloy and the stress distribution in the file, it can be claimed that the file was subjected to the forces applied in the transition phase, i.e austenite-to-martenrite phase. Based on Fig. 6, the amounts of torsional forces increase towards the top of the file. Furthermore, the amounts of forces applied from the center towards the file's outer walls are increased so that the maximum amounts of torsional force enter the depth of the flutes. Considering how the flexural and torsional stresses are distributed in the files, it can be concluded that in all files the maximum number of torsional stresses is applied in 2 to 3 mm of the file tips. Additionally, the highest amounts of flexural stresses are applied at the depth of the flutes and close to the winning edges. Moreover, a comparison of the highest values of Von Mises Stress (VMS) in the files demonstrates that the highest values of flexural stresses are seen in the Edge endo file and the lowest values in the Vortex Blue file (Table 1).

Table 2 indicates the mechanical properties applied to the computer models in this study. In addition, the highest and lowest amounts of flexural stress are seen in the Edge Endo file Vortex Blue file, respectively. The two main forces that cause rotary files to fail are flexural and torsional forces. The torsional failure occurs when the instrument is locked in the channel while the shank continues to rotate, and the bending failure happens due to the repeated use of the file and its fatigue. Various

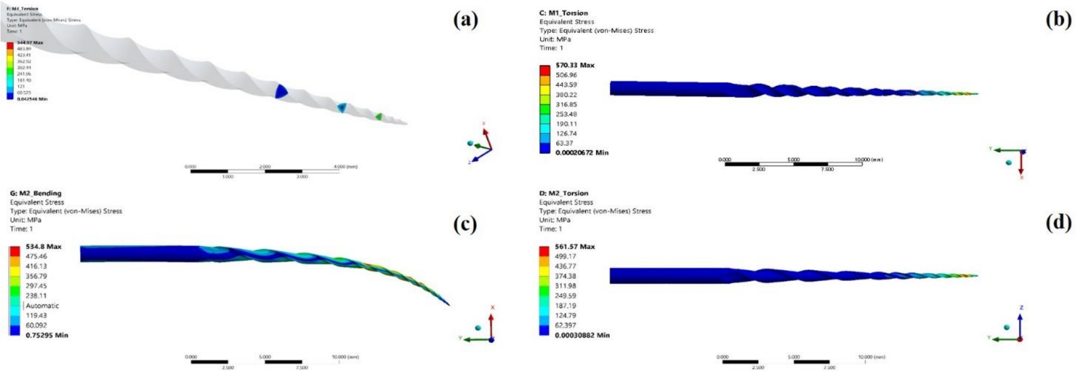

Fig. 6. Distribute torsion stresses in the a) Vortex blue file (file length view), b) Hyflex EDM file (longitudinal view of the file), c) in the One Curve file (longitudinal view of the file), and d) One Curve file (longitudinal view of the file).

factors affect the mechanical properties of rotary files and their resistance to failure. Some of these factors include the properties of the alloy used in its fabrication, physical properties such as cross section, number of flutes, and pitch length. This study was conducted using FEA and the purpose was to evaluate and model the geometry of four different rotary files including VortexBlue (Dentsply), Edge File (Edge endo), HyFlex EDM (coltene), and Onecurve (MICRO MEGA) with the same tip diameter of 0.25 mm, file length of 25 mm, and convergence of 0.06. In order to apply the bending force, the tip of the file was bent by 3.8 mm and the file was rotated by 22° to apply the torsional forces. The extent and manner of distribution of Von Mises Stress (VMS) during torsional and flexural forces was evaluated in all the files. The success of any dental procedure depends primarily on the dentist and secondly on the materials and tools used [14, 19]. The introduction and application of NiTi in rotary systems has greatly simplified the formation of the root canal system. NiTi superelasticity allows it to be used in continuous rotation and even reduces the risk of channel path transport in curved channels during clearing and shaping the channel. However, breaking the file due to fatigue is a major concern cycle. Repeated traction and compression cycles, particularly in channels with extreme curvature, cause cumulative microstructural changes which eventually lead to instrument breakage. Therefore, the key issue for the dentist is to select a rotary file system that, apart from being flexible enough to retain the anatomy of the canal while still being strong enough to prevent fracture inside the canal. Omar et al. [34] showed alower value in their studies. In addition, Peters et al. [45] stated that the cross-sectional area of the file is a crucial parameter that affects the tool life, since the cross-sectional shape of the angles that strike the dentin walls, when cutting directly, impacts the shear efficiency of the instrument [45]. Hansen et al. [48] conducted an *in vitro* study on different generations of Edge Endo files and compared them with different rotary file generators. The results of this study indicate that the Vortex Blue file is stronger (more resistant to torsional stress) than the Edge Endo X3 file, which can be attributed to having a larger cross-section. Further, the results illustrate that the highest amounts of flexural stresses (from highest to lowest) were seen in Edge File (620.85MPa)> Hyflex EDM (570.33MPa)> One curve (561.57)> Vortex blue (544.37) (see Fig. 4 (a-b), Fig. 5 (a-e), Fig. 6 (a-d)), respectively. The Edge File file has a drastically different distribution of flexural stresses than other files, making it stiffer. However, the values of these stresses are lower in the Vortex Blue file, rendering it more flexible than other files. Furthermore, in all four studied

Table 2. Mechanical properties applied to computer models [14, 19].

Maximum force transformation (MPa)-End point	Maximum force transformation (MPa)-Start point	Elastic modulus (GPa)	Poisson ratio
755	504	36	0.3

files, the highest accumulation of flexural stresses was observed at the winning edges and close to the depth of the flute. In files with uniform cross-sections, such as Vortex Blue and regular Edge files, the distribution of these stresses is uniform. However, in the Edge file the amounts of VMS are higher, which can be related to its triple helix cross section. The concentration and accumulation of stress in these areas increases the amount of fatigue and creates points with less breaking resistance. In areas with higher flexural stress peaks, the file is more likely to fail. The torsional and flexural properties of rotary files, as well as the proper design of their cutting blades, have enabled them to be used with rotary handpieces [65-68]. Rotary motors are continuously rotating and have one-way torque. This exposes the instrument to constant and changing stresses depending on the anatomy of the canal and the hardness of the cut dentin; thus, it is paramount that the applied instrument is both flexible and strong [2]. Studies have shown that files with more flexibility shape the channel path better due to their caoacity to be more centered and minimize deviations [19-30]. NiTi memory alloy is a suitable biomaterial for utilizing in root canal files due to its capacity to tolerate high elastic deformation and biocompatibility. Having austenitic structure, NiTi files can easily go through the sharp bends of the root canal owing to their superelastic properties and martensitic transformation under stress. Thus, they are superior to the files made of stainless steel. Endodontic files rotate inside the canal, causing tensile and compressive forces to fluctuate. These variable loads over time lead to periodic fatigue of the tool and are regarded as an important factor in file breakage [67-72]. These stress values are less intense in the Vortex Blue file and are more evenly distributed. Additionally, based on the results of the study, the highest amount of torsional stress is observed in 2 to 3 mm at the tip of all 4 files, which was confirmed by Arbab-Chirani et al. [3]. The highest values of torsional stresses were found in Edge File (573.6MPa)> Hyflex EDM (570.33MPa)> One curve (561.57MPa)> Vortex blue (544.37MPa), respectively. The Vortex Blue file has a cross-section of a convex triangle with higher cross-sectional inertia than other files, making it more torque-resistant. Researchers have indicated that the larger the cross section of the file, the higher the torsional strength of the file. In other words, less stress is accumulated during cutting in the file. This obtained result is confirmed by other studies on the corrolation between the cross section diameter and torsional resistance of files [51-56]. Ahamed et al. [28] introduced an optimal model for ramdley flexural stresses that had different cross-sectional levels along the file. However, in the present study, convex triangular cross-sectional files performed better against flexural and torsional stresses throughout the file length [69-79].

CONCLUSION

Many file developers strive to create a product that is both robust enough to withstand torsional forces and flexibile enough to follow the anatomy of the canal. New systems have been developed from NiTi rotary tools that have more power and flexibility. The more flexibile and strong the file, the less likely it is to break while retaining the proper anatomy of the canal. Flexibility can be as important as strength; nonetheless, flexibility is usually sacrificed in favor of strength. Although the files investigated were from different brands and systems, they were selected for comparison in this study because they have approximately the same diameters and convergences. In addition, the torque applied to the instrument and its resistance to torsion are affected by these parameters. This is why most research on tools considers these two factors. It should be noted that as the geometric properties of the files change, their mechanical behavior under different forces may also vary. The obtained results demonstrate that the files with the highest values of torsional and flexural stresses in descending order are: Vortex Blue <One Curve <Hyflex EDm <Edge File. The highest amounts of stress on the Edge File can be related to its triple helix cross section, since the geometry of this file is such that the weaker areas create the most stressful concentrations. The obatained results indicate that the flexural and torsional properties of the Vortex Blue file are better than other files; therefore, it can be concluded that this file can be used in narrower, more curved channels, while the Edge File is recommended for wider and less curved channels. The values of flexural and torsional stresses in both Hyflex EDM and One Curve files are very close, and due to the results of their comparison with other brands, their use in medium curvature channels is highly recommended. Comparing the results of experimental studies with computer studies can be a validation method for FEA studies. Numerical simulations with an appropriate behavioral model can facilitate comparisons of existing instruments.

These simulations may also be used to compare and design new instrument geometries in less time and at a lower cost. Moreover, analyses can predict the properties of the instruments by changing the geometric shape and type of alloy used. In order to better understand the properties of the tools, their failure risk and lifespan should be evaluated before processing the prototype.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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