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ORIGINAL ARTICLE

Modeling viscoelastic behavior of periodontal ligament with nonlinear finite element analysis

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Abstract *Background/purpose:* The function and role of periodontal ligament (PDL) are of interest in a number of fields. Due to the complexity of the geometry and the impossibility of obtaining specimens, the mechanical properties of PDL remain uncertain. The object of this study was to investigate the viscoelastic behavior of PDL by means of nonlinear finite element analysis.

Materials and methods: In order to consider nonlinear force-displacement behavior, we proposed a finite strain viscoelasticity material model to represent PDL tissue. The strain energy consists of two kinds. The first is nonlinear in time, called viscoelasticity, and the other is geometrically nonlinear, called hyperelasticity. We obtained the material properties by retrograde calculation based on Ross's experiments.

Results: The results demonstrate that viscoelastic properties mainly result from volumetric changes. The sources of volumetric change are fluids and the vascular system. Second, by combining the nonlinear geometric properties, we can simulate nonlinear load-displacement relationships. We found that the finite strain viscoelastic model can model both nonlinear load-displacement relationships and nonlinear time-displacement relationships.

Conclusion: The nonlinear finite strain viscoelastic model can simulate both the creeping behavior and nonlinear load displacement behavior of teeth, and may be the best-fitting model for understanding the mechanical properties of PDL.

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Introduction

An understanding of how periodontal ligament (PDL) functions is the missing link in dental biomechanics, and an

accurate understanding of how PDL functions could have multiple applications in several areas of dentistry. For example, in fixed and removable prosthodontics, the concern is how forces transfer from a bridge or denture to the masticatory apparatus; this knowledge would be helpful to those who are trying to model the human masticatory apparatus.^{1,2} Moreover, orthodontists are concerned with the forces needed to move teeth that are mediated through PDL, and the relation of tooth mobility and periodontal disease is a concern of the periodontist.

PDL is connective tissue that connects the teeth to the alveolus. It is generally accepted that the functional role of PDL is primarily tooth support. However, theories of how PDL supports teeth range from the classical hammock theory to the viscoelastic theory. According to the classical view of tooth support mechanism, PDL is only a suspensory ligament. However, research has shown that unstressed collagen fibers are wavy,^{3,4} and also that the organization of periodontal collagen reflects the magnitude and direction of the masticatory forces.^{5–9} In contrast to the tensional hypothesis, Wills and Picton's^{10–12} results showed that the alveolar margins dilated under axial loading. They revealed that the periodontal tissues acted as a compressive system for resisting axial loads. At the same time, the convergence of the alveolar margins was predicted as a tensional system. One possible tooth support mechanism could be a combination of the tensional and compressive hypotheses, that is, that the tooth is supported by both compressive and tensional reactions in different parts of the PDL.⁷

Reported *in vivo* experimental data directly related to the mechanical properties of PDL are limited and almost exclusively employ a linear elastic model. Some of them consider the time-dependent effect. However, obtaining material constants for a time-dependent model is difficult and not sufficient to model the behavior of PDL completely. A more thorough mathematical model is needed to represent the mechanical behavior of PDL.

The purpose of this research was to explore the mechanical properties of PDL using reported data on human and animal tooth movement, to calculate the material constants with finite element analysis. In this paper, we propose a series of models describing the relationship between the functions and properties of PDL to explore its viscoelastic behavior, and thereby to find out which material model most accurately represents well-known PDL behavior.

Materials and methods

Constructing finite element geometry models

In this research, a maxillary central incisor was embedded and sectioned into 19 slices for construction of a three-dimensional finite element mode. The three-dimensional finite element model, comprising a maxillary central incisor, pulp chamber, cementum, PDL, cortical bone, and cancellous bone, consisted of 3772 nodes and 3721 isoparametric eight-node solid elements. The construction of the finite element model began with the design of a geometric model of the tooth, which we based on the

dimensions of a sample tooth and the general morphology of the maxillary central incisors from Wheeler's *Dental Anatomy, Physiology, and Occlusion*.¹³ We simulated PDL as a 0.25-mm-thick layer and divided it into four-layer elements. The alveolar bone was modeled according to the standard size reported in relevant research. We used the software ABAQUS (ABAQUS Inc., Rising Sun Mills, Providence, RI, USA) 5.8.14 and I-DEAS (Siemens PLM Software, Plano, TX, USA) 7.0 to construct the finite element model.¹⁴ The loading and boundary conditions were the bottom of the alveolar bone to be fixed and the asymmetric sides, as shown in Fig. 1.

Material properties

The tissue properties of PDL, dentin, enamel, pulp chamber, cementum, cortical bone, and cancellous bone based on previous studies are shown in Table 1. We obtained the material properties of PDL from previous work and back-calculations. Although the data may not be exactly correct, the tendency of the curve appears the same, and the results of mastication simulation are relatively reliable.

PDL mechanical Model 1—nonlinear time effect only

The mechanical behavior of PDL tissue is still uncertain, and the most accepted mechanical explanation is the viscoelastic hypothesis. The basic hereditary integral formulation for linear isotropic viscoelasticity can be written as the following form:

$$\sigma(t) = \int_0^t 2G(\tau - \tau') \dot{e} dt + I \int_0^t 2K(\tau - \tau') \dot{\phi} dt \quad (1)$$

where e and ϕ are the mechanical deviatoric and volumetric strain, K is the bulk modulus, and G is the shear modulus, which are functions of the reduced time τ and denote differentiation with respect to t . The relaxation functions $K(t)$ and $G(t)$ can be defined individually in terms of a series of exponentials known as the Prony series:

$$K(t) = K_\infty + \sum_{i=1}^N K_i e^{-\tau/\tau_i}, \quad (2)$$

$$G(t) = G_\infty + \sum_{i=1}^N G_i e^{-\tau/\tau_i}, \quad (3)$$

where K_∞ and G_∞ represent the long-term bulk and shear moduli. By fitting the Prony constants (K_i , G_i , τ_i^k) of the above bulk and shear relaxation functions.

To find out which time effect is the most likely source of the creep or relaxation behavior of PDL, we used two material assumptions to fit Picton's tooth-displacement experiment data. One is the volumetric time effect only, and the other is the shear time effect only. Model 2 is a linear volumetric viscoelastic model, and Model 3 is a deviatoric viscoelastic model. The relaxation parameters can be defined directly according to specifications of the Prony series parameters. The material constants of PDL can be obtained from back-calculation of Picton's experiment.⁸

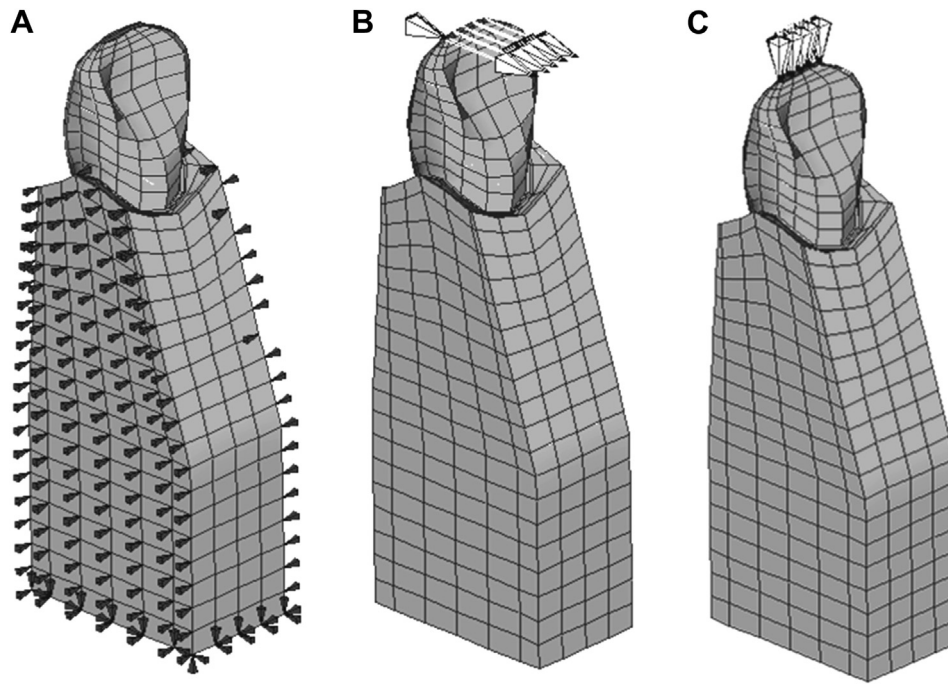


Figure 1 Boundary conditions and loading conditions: (A) boundary condition, (B) lateral loading condition, and (C) intrusive loading condition.

PDL mechanical Model 2—nonlinear time effect and nonlinear geometric effect

To thoroughly consider the mechanical behavior of PDL, we needed to consider both nonlinear time and nonlinear geometric effects. A linear elastic model, linear isotropic viscoelastic model, and finite strain viscoelastic model were used to fit the tooth load–displacement curves, including the nonlinear time effect and nonlinear geometric effect.

In all cases, elastic moduli must be specified to define the rate-independent aspect of the material’s behavior. The elastic material behavior is defined as small-strain linear elastic behavior, and large-deformation behavior is defined by hyperelastic material behavior.

For hyperelastic material behavior, we applied the relaxation coefficients to the constants that define the strain energy function. The strain energy function in reduced polynomial form is

$$U = \sum_{i=1}^N C_{i0} (\bar{I}_1 - 3)^i + \sum_{i=1}^N \frac{1}{D_i} (J - 1)^{2i}, \tag{4}$$

where U is the strain energy per unit of reference volume, C_{i0} and D_i are material parameters, and \bar{I}_1 is the first deviatoric strain invariant defined as

$$\bar{I}_1 = \bar{\lambda}_1^2 + \bar{\lambda}_2^2 + \bar{\lambda}_3^2, \tag{5}$$

where the deviatoric stretches $\bar{\lambda}_1 = J^{-\frac{1}{3}} \lambda_i$, J is the total volume ratio, and λ_i are the principal stretches.

C_{i0} governs the shear behavior of the material, and D_i determines the compressibility of the material. To model the time-dependent behavior of the tissue, the coefficients in the energy function formula (4) can be written in the form of an exponential series:

$$C_{i0}(t) = C_{i0\infty} + \sum_{k=1}^N C_{i0k} e^{-\tau/\tau_k}, \tag{6}$$

$$D_i(t) = D_{i\infty} + \sum_{k=1}^N D_{ik} e^{-\tau/\tau_k}, \tag{7}$$

and the energy function can be presented in the form of a convolution integral.

Fitting of creep curve

Based on the above assumption, we used these four models to fit the creep test data to explain the mechanical behavior of PDL. The creep curve fitting is based on an experiment by Ross et al.¹⁶ and the corresponding loading condition is to apply a 0.05 N lingually directed load and maintain it for 2.5 seconds before releasing it.

Table 1 Material constants of finite element model.

Tissues	Modulus of elasticity (Mpa)	Poisson’s ratio
Enamel	84,000	0.31
Dentin	18,600	0.31
Cementum	18,600	0.31
Cortical bone	13,700	0.3
Trabecular bone	1,370	0.3
Pulp	0.01	0.49

Fitting of nonlinear load–displacement curve

The nonlinear load–displacement curve fitting is based on an experiment by Parfitt¹⁷—the axial force/movement curve of the same upper incisor tooth in the evening. The loading condition is to apply an increasing force to 2.5 N within 2.5 seconds.

Determination of material constants for PDL tissue

For Models 2 and 3 the material constants are obtained from the curve fitting of the creep curve, and for Model 4 the mechanical constants are obtained from the creep curve and the nonlinear load–displacement curve.

To obtain a good agreement between theory and experiment in Model 4, it is necessary to obtain third-order terms in the energy function (4). Then for $N = 3$

$$U = C_{10}(\bar{I}_1 - 3)^1 + C_{20}(\bar{I}_1 - 3)^2 + C_{30}(\bar{I}_1 - 3)^3 + \frac{1}{D_1}(J - 1)^2 + \frac{1}{D_2}(J - 1)^4 + \frac{1}{D_3}(J - 1)^6 \quad (8)$$

It is impossible to tell them apart from only one nonlinear load–displacement curve. We assume that the volumetric part is controlled by the viscoelastic model, Prony's constants, and the constants, D_i , are first chosen to be constant. Only the constants of the deviatoric part need to be decided by curve-fitting.

Results

Creep curve fitting

When fitting the creep curve, all other models except for the linear elastic model can fit the creep curve well, with the exception of unloading, as shown in Fig. 2. For the period of unloading, the speed of decay is quicker than the real one.

Nonlinear curve fitting

Only finite strain viscoelastic behavior can fit the nonlinear curve well, as shown in Fig. 3. The nonlinear load displacement characteristic of tooth movement is due to the different behavior of PDL under different loading

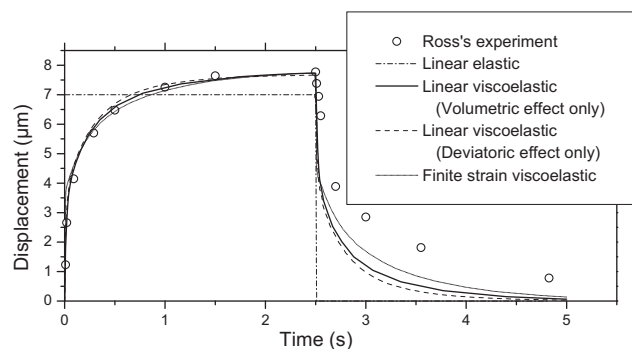


Figure 2 Curve fitting of the creep test data.

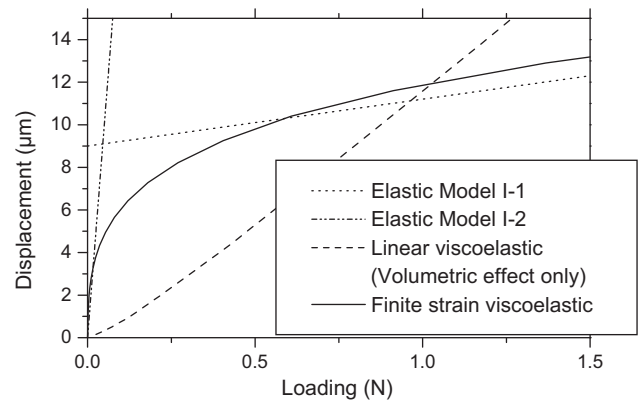


Figure 3 Nonlinear curve fitting.

magnitudes. The corresponding material constants from the curve fitting of the linear elastic model are shown in Table 2. Linear isotropic viscoelastic models, both volumetric and deviatoric, are shown in Table 3, and finite strain viscoelastic material is shown in Table 4. The magnitude of Young's modulus of PDL under a large load is within the same range as in previous studies. This is why the Young's modulus of PDL varies dramatically in previous reports.

Comparison between different PDL material models

The assumptions and results for all four models of PDL tissue are listed in Table 5. Only the volumetric finite strain viscoelastic model can simulate nonlinear load–displacement behavior, creep behavior, and pressure stress change in normal PDL.

Discussion

In this study, we present and summarize mathematical models of PDL tissue deformation behavior (Table 5). The tissue exhibits nonlinear stress–strain relations as well as a strong dependence between stress and time. Only the finite strain viscoelastic model can represent both the creep behavior under constant load magnitude and nonlinear load displacement behavior. This is the first time both these nonlinear effects of PDL have been considered together in both a mathematical model and finite element simulation.

The finite strain viscoelastic model is a nonlinear elastic material model depending both on time and geometric effects. The name “finite strain” is used to describe the behavior of material under large deformation, and the

Table 2 Linear elastic material constants for Model 1.

Model 1—elastic		
E (MPa)	Small load (F = 0.05 N)	Large load (F = 2.5 N)
	0.005	0.5
ν	0.49	0.49

Table 3 Linear isotropic viscoelastic material constants for Models 2 and 3.

	Volumetric viscoelastic				Deviatoric viscoelastic			
E (MPa)	0.23				0.087			
ν	0.49				0.49			
Prony constants	τ	0.0025	0.1	0.5	τ	0.0025	0.1	0.5
	K	0.155	0.4	0.15	K	0	0	0
	G	0	0	0	G	0.91	0.05	0.005

material models used to represent such large-deformation behavior are usually called hyperelastic models or hypoelastic models. In the finite strain viscoelastic model, we used hyperelasticity to simulate the nonlinear stress–strain relation and viscoelasticity to stand for the nonlinear stress–time relation or nonlinear strain–time relation.

It is well known that the mechanical behavior of PDL is time-dependent. From the observation of a histologic section of PDL and the theories of continuous mechanics, we can assume that there are two possible sources of tooth creep behavior. One is the volumetric effect that represents the free fluid in PDL flowing between the spaces in PDL¹⁵ and the alveolar bone; the other is the deviatoric effect that means PDL material continuously changes its shape under intrusive loads as time increases. According to these two opposite assumptions, we built up two models: a volumetric viscoelastic and a deviatoric viscoelastic model. With the aid of Prony's constants for calculation and the loading period of the lateral movement of teeth in Ross's results,¹⁶ it is possible to model the creep behavior of PDL. Both these models can simulate creep behavior correctly, and the corresponding material constants are acquired from back-calculation, as shown in Tables 3 and 4.

Since all material models that contain the nonlinear time effect can simulate the creep behavior, the source of creep in PDL is still uncertain. The two major possible creep sources come from fluid dispersion and distortion of PDL itself. From the pressure stress change pattern during loading and unloading, we can see that the pressure stress pattern of the volumetric effect model is more like the fluid pressure changes in PDL of the mandibular canine tooth of dogs reported in Walker et al's results,¹⁸ as shown in Fig. 4. The pressure stress change in PDL of the volumetric model matches the P-response (positive pressure peak), and the pressure stress change in the deviatoric model is the typical S-response (sustained pressure) in Walker et al's report.¹⁸ The P-response stands for the behavior of normal or undamaged PDL, while the S-response represents the behavior

of damaged PDL. It can be concluded that the initial source of creep comes from the volumetric time effect, and the free fluid movement between the PDL and the surrounding tissues. The free fluid system in PDL includes the blood and unbound tissue fluid. However, as most of the liquid in PDL is bound, only the fluid in the blood vessels can flow freely.¹⁹ Therefore the most likely source of creep is the vascular system.

According to histological observations, the major components of PDL are water, proteoglycans, and glycosaminoglycans.²⁰ In the initial stage of tooth movement, it is believed that the collagen fibers are still wavy⁴ and are not subjected to medial loading such as orthodontic and mastication forces. There is no time for a biochemical process to change the structure of PDL. Therefore, we believe that the mechanical behavior of normal PDL tissue is dominated by a bulk time effect in the initial stage of loading.

The curves of load displacement and recovery for a single tooth have been described many times. The nonlinearity of the load–displacement curve is usually explained as the tooth floating in unstressed PDL. In the initial stage, the force causes the fluid, mostly in the blood vessels, to be displaced,^{21,22} so that the tooth moves quite freely. As the load increases, the principle fibers progressively come under tension.^{10,23} In the second stage of loading, the force is transmitted to the alveolar bone, and causes both displacement of the socket and distortion of the alveolar bone. In conclusion, PDL is designed to withstand the large but short-acting forces that occur in mastication, which cause relatively small but long-term effects on the tooth's position in the socket. While unloading, mechanisms in PDL generate a continuous net extrusive force in the order of 1 g. The tooth position in the alveolar bone is determined by the interplay of these opposing mechanisms in the PDL. However, there are no direct observations or evidence to prove this proposition.^{10,12,24–26}

The linear volumetric viscoelastic model is a geometric linear model and can be used to simulate the initial tooth movement; however it fails to simulate nonlinear load displacement related to tooth movement. The source of the nonlinearity comes from the unstressed collagen fibers and the nondispersed fluid, which make the tooth more flexible in the small loading period, like rubber. In order to consider the nonlinear force–displacement behavior, we use a finite strain viscoelasticity material model to represent PDL. The strain energy form consists of two kinds. One is volumetric and the other is deviatoric. The curve fitting results are shown in Fig. 3. The volumetric viscoelastic model can simulate the nondispersed fluid, and the hyperelastic model can simulate the unstressed collagen fiber. Combining these two models, we obtained a finite

Table 4 Finite strain viscoelastic material constants for Model 4.

	Volumetric finite strain viscoelastic			
N	1	2	3	
C_{i0}	0.01	5	1000	
D_i	2	0.01	0.001	
Prony constants	τ	0.0025	0.1	0.5
	K	0.155	0.4	0.15
	G	0	0	0

Table 5 Comparison between different periodontal ligament (PDL) material models.

Model type	Assumptions		Results				
	Nonlinearity		Load–displacement behaviors simulation		Stress distribution		Pressure stress change in PDL
	Time	Geometry	Creep	Nonlinear	Crown	Root	
Elastic			Yes		Yes		
Volumetric viscoelastic	Yes		Yes		Yes	Yes	Normal PDL
Deviatoric viscoelastic	Yes		Yes		Yes		Damaged PDL
Finite strain viscoelastic	Yes	Yes	Yes	Yes	Yes	Yes	Normal PDL

strain viscoelastic model, which can simulate both the time nonlinearity and the geometric nonlinearity. In other words, the finite strain viscoelastic model can simulate both the creep aspect and the nonlinear load–displacement aspect of tooth movement.

The finite strain viscoelastic model matches the experimental results very closely during the loading period. However, the downward tendency of the unloading creep curve is quicker in reality than it appears in the experimental data. The reason for the bad curve fit during the unloading period is that the rate of creep under unloading is

much smaller than it is under loading. The bad curve fit is not important because the stress magnitude decreases by unloading as time passes and will not cause any tissue damage.

It is noteworthy that when PDL material is assumed to have a shearing effect viscoelasticity only and the tooth is subjected to an axial intrusive load, the stress pattern in the bone will increase with time, and the stress pattern in the tooth's root will also change with time. It can be said that a sustained load will lead to destruction of the alveolar bone. Observing changes in the stress pattern as time

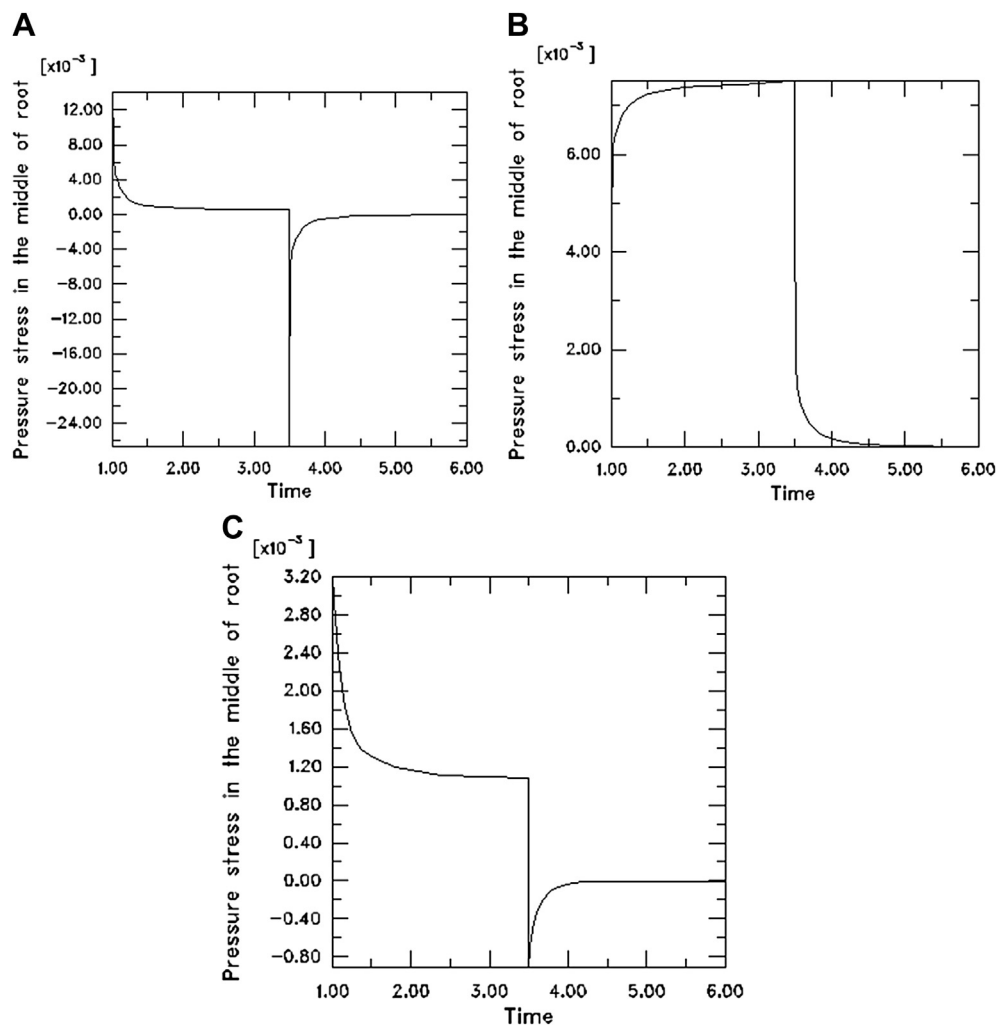


Figure 4 Periodontal ligament pressure stress in the middle of root for (A) the volumetric viscoelastic model, (B) the deviatoric viscoelastic model, and (C) the finite strain viscoelastic model.

increases indicates the sensitivity of periodontium when the tooth is subjected to a different loading history. These viscoelastic properties are used to absorb energy, change the stress pattern of the tooth, and reduce the stress magnitude both in bone and in the root of the tooth in the initial stage. The advantages of the creep behavior of PDL are reducing stress magnitude and dispersing the concentration of stress around PDL.

In Fig. 2, showing the creep curve fitting, if PDL is assumed to be a linear elastic material, we find that it cannot be used to simulate the nonlinear time effect on teeth. The elastic model is insufficient to describe the material properties of PDL, as well as all other soft tissues. Young's modulus used here is obtained by curve fitting of the nonlinear load–displacement curve of the tooth under a small load and a large load, respectively. The studies of PDL that use elastic material cannot simulate all tooth movement behavior or the changes of stress distribution patterns around the PDL. On the other hand, the stress patterns on the tooth crown are almost the same as time increases. According to Saint-Venant's principle, a theory of elasticity, no matter what the conditions of loading in the PDL are, the stress patterns will be the same. If the research focuses on the crown, the influence of time-dependent properties in PDL are minimal, but it is still necessary to pay attention to changes around the roots of teeth.^{26,27}

More experimental work is required to verify the validity of the assumptions used for model derivation as well as the numerical values of material constants for PDL. Further research is still required to determine material constants that would be able to distinguish between volumetric and deviatoric effects, a project to which we will devote ourselves in the future. The role of PDL in tooth support is of interest to a number of fields. If the material behavior of PDL is known, it will be easier to predict the behavior of orthodontic tooth movement, which will help in the dentine implant design process. Furthermore, an extraoral experiment could be set up using material with the same material properties as PDL. With this experiment setup, all experiments relating to PDL, such as exploring the mechanics of root fracture, could be done in the laboratory. This would improve the biomechanics of dentine development.

In this paper, we have proposed that the finite strain viscoelastic model can accurately simulate the behavior of PDL, and the source of creep in PDL comes from free fluids. As for acute force or chronic force and extraoral experiment design, much improvement is needed. If all these challenges can be met, we can arrive at a comprehensive understanding of the biomechanical behavior of PDL.

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