Velocity and wall shear stress of 18% EDTA irrigation solution flow in the removal of $Ca(OH)_2$ with computational fluid dynamic analysis

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ABSTRACT

Introduction: Ethylene Diamine Tetra Acetic Acid (EDTA) 18% irrigation solution is one of the chelating agents that able to remove calcium hydroxide (Ca(OH)2) from the root canal wall. Failure of root canal treatment can be caused by the presence of residual calcium hydroxide in the root canal wall, thus blocking the bond between the medication and root canal filling material with the root canal wall. This study was aimed to observe the EDTA 18% flow in removing the Ca(OH)2 using CFD analysis. **Methods:** This research was descriptive. Cleanliness of the root canal wall from Ca(OH)2 medicament using EDTA 18% irrigation was analysed using the CFD method with test specimens in the form of resin blocks made according to the characteristics of the root canal. The irrigation needle used was side-vented with a position of 3 mm from the apical tooth. Stage analysis of root canal geometry was performed using Computational Fluid Dynamics (CFD) analysis to observe the characteristics of irrigation solutions in root canals in 3D. **Results:** The streamlined characteristics of EDTA 18% irrigation solution showed a unique behaviour due to the features of the side-vent shaped irrigation needle. Irrigation flow in the crown area of the inlet (side-vented irrigation needle) showed low velocity so that the fluid flow when exiting the inlet was more towards the apical than the outlet (root canal orifice). **Conclusion:** Velocity and wall shear stress of EDTA 18% showed the results validation conformity between experimental and CFD, that the maximum velocity of EDTA 18% is 19 ms-1 and EDTA 18% wall shear stress is 1.56 KPa for calcium hydroxide removal observed from the CFD study.

Keywords: Computational fluid dynamics, EDTA 18%, calcium hydroxide (Ca(OH)2), velocity, wall shear stress

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INTRODUCTION

Factors that influence the success of root canal treatment are biomechanical preparation, root canal sterilisation and proper root canal filling. Biomechanical preparation consists of instrumentation and irrigation stages. Root canal irrigation aims to dissolve tissue, kill microorganisms, remove debris and smear layers, cleanse root canals, and lubricate during root canal preparation.[1,2]

$Ca(OH)_2$ can neutralize endotoxins bacterial, stimulate healing processes in periapical tissues, good antimicrobials, and can stimulate root formation at imperfect root closure.[3,4] Residue of $Ca(OH)_2$ medicament must be removed entirely from the root canal wall prior to the filling action to prevent interference between the filling material with the root canal wall. $Ca(OH)_2$ medicament can cause dentinal tubule closure of the root canal so that the filling medication does not penetrate the dentinal tubules so that it interferes with the bond of the medication to the canal wall, and will eventually cause the failure of root canal treatment.[4,5] EDTA 18% solution is a solution that functions as a chelating agent used as lubricant root canals and irrigation solutions to clean debris and inorganic smear layers.

Computational Fluid Dynamics (CFD) analysis is an analysis that studies how to predict fluid flow, heat transfer, chemical reactions, and other flow phenomena in mathematical equations.[8-10] An exhaustive understanding of fluid flow characteristics is difficult to obtain using an experimental approach but can be obtained easily with the CFD approach.[12] CFD applications have now been widely used in the field of dentistry in studying irrigation systems on root canal treatment.[13,14] This study was aimed to observe the EDTA 18% flow in removing the $Ca(OH)_2$ using CFD analysis.

METHODS

This descriptive research begins with the making of test specimens in the form of one single customised root canal block resin with geometric characteristics by the study of Boutsikouis et al.[12] The fabrication was performed through the analysis phase of geometrical frustum cone shape of the root canal, with root canal length of 18 mm, root canal orifice diameter of 1.57 mm, root canal apical diameter of 0.45 mm, and taper of 6.2% (Figure 1).[15,16]

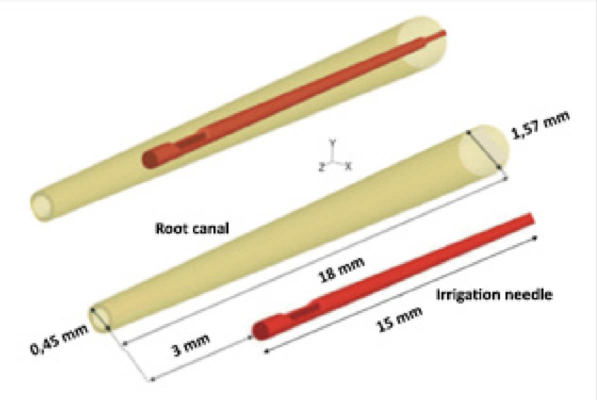

Figure 1. Design of the shape and size of root canal test specimens[17]

$Ca(OH)_2$ medicament paste was applied to a customised block resin root canal. Irrigation of EDTA 18% solution using a 30G side-vent irrigation needle, with a working length of less than 3 mm from the root canal length for 19 seconds using a syringe pump with a flow rate of 0.26 mL / s. The EDTA 18% irrigation process for removal of $Ca(OH)_2$ was recorded with the Super Slow Motion NXCAM Full HD Camcorder (Sony™ NEX-FS700R). Observations were made based on the pattern of particle movement in the root canal for 19 seconds.

The initial preparation of the CFD research was the reconstruction of the root canal geometry by forming a geometric CAD model of the root canal following the size formed using SpaceClaim© Software (Figure 2). This size was consistent with root canal test specimens used in experimental studies.

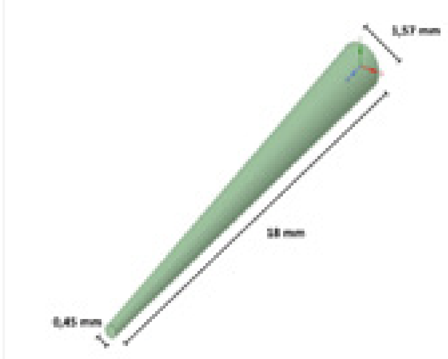

Figure 2. CAD geometric model design of root canal

The second stage was the analysis of the 30G side-vent needle geometry (Prorinse Dentsply™) obtained from the results of scanning micro-computed tomography (Micro-CT). Irrigation needles are arranged on plasticine with 20 mm of the tip of the needle facing upwards, and the Micro-CT was carried out for 3 hours. The scanning results were reconstructed into 3D shapes and verified with the external diameter size of the Dext needle (0.30 mm) as by literature[16] and formed into CAD using the Spaceclaim© Software. The needle length was adjusted with the simulation root canal length, reduced by 3 mm, which was precisely 15 mm. Irrigation needles would be placed at a distance of 3 mm from the apical edge, positioned in the middle of the root canal, and keep static.

The third stage was the formation of mesh and flow domains, namely the surface of the inlet, outlet, and root canal walls, that were constructed using Pre-processor CFD Ansys Meshing Software 17.1. The formation of the mesh consisted of the stages of pre-processing, processing, and post-processing. The fluid flowed into the simulated domain through the inlet (side-vent irrigation needle) and exited through the outlet (root canal orifice) as a result of atmospheric pressure given to the outlet.

The pre-processing phase began with the transfer of the CAD geometric model of the root canal and the irrigation needle; then the computational domain was formed in the geometric model of the root canal. Formation of mesh models on the outer surface and volume in root canals and irrigation needles. Evaluation and improvement of mesh quality. Output: mesh, surface boundary, and epithet.

The processing phase started by inputting mesh with data on the name of the chemical structure of EDTA 18% fluid and $Ca(OH)_2$, the physical and chemical properties of the fluid (density, viscosity, and pH), the result of a chemical reaction to $Ca(OH)_2$. Determination of fluid flow equation models and physical models, numerical parameters, numerical schemes. Analysis of EDTA 18% solution and root canal paste filled with $Ca(OH)_2$ medicament and the needle filled with an irrigated solution. The effect of gravity was included in the simulation because of the potential energy of the flow. Laboratory analysis was carried out to obtain density, viscosity, and pH values from EDTA 18% solution, and $Ca(OH)_2$ paste. Fluid density was measured using a pycnometer, while fluid viscosity was measured using the falling sphere viscometer.

CFD program was run, and the growth of errors was monitored. The results were simulated, and irrigation of EDTA 18% towards $Ca(OH)_2$ in the root canal process animation was made using Ansys-Fluent Software. The post-processing phase after animation was obtained by displaying domain and mesh geometry, flow pattern analysis (streamlined and vector), contour velocity, pressure contour, 2D image dimensions, 3D animation video; then observation output and velocity calculation (contours, vectors, and streamlined), wall shear stress, volume fraction of $Ca(OH)_2$ medicaments and EDTA 18% solution and validation of the results of CFD research on experimental research.

Calculation of CFD simulation was performed using timestep for 10^{-3} seconds given in real time flow before 0.1 seconds. The maximum scale of the convergence criterion was set at 10^{-4}. Volume and velocity fractions were monitored every timestep to ensure adequate convergence. Computation was performed using a computer with Intel™ Xeon Processor 12 Core @ 2.00 GHz 128GB DDR3 ECC RAM 64-bit Operating System. The flow area was calculated to see flow patterns, velocity size, wall shear stress, and fluid volume fraction. Lagrangian particle tracking was carried out at the post-processing stage. The tracking was carried out on the path of massless particles in the flow domain between the inlet to the outlet.

The results of this study were validated with the results of CFD research in the form of volume fraction of fluid movement patterns in the root canal wall. The study was conducted at the Conservative Dentistry Specialist Program Clinic of the Faculty of Dentistry Universitas Padjadjaran; Computer Laboratory of the Faculty of Dentistry Universitas Padjadjaran; Physics Laboratory of Bandung Institute of Technology; Pharmacy Laboratory of Bandung Institute of Technology; and Aero Gas Dynamics and CFD Laboratory of the Faculty of Mechanical and Aerospace Engineering, Bandung Institute of Technology. Analysis of validation and CFD experimental results data was used graphically to analyse data.

An experimental study was carried out using customised block resin specimens (Figure 1). An EDTA 18% solution was injected into the root canal containing the $Ca(OH)_2$ medicament using a 30G side-vent irrigation needle and syringe pump with a flow rate of 0.26 mLs^{-1}. The process was recorded using a Super Slow Motion Camcorder (Sony™ NEX-FS700R) 960 frame s^{-1} for 19 seconds supported with a 105 mm macro lens, and a super bright 5400K LED panel. The results of this study were validated with the results of CFD research in the form of volume fraction of fluid movement patterns in the root canal wall. The results of the CFD study observed in this study were the volume fraction in the cross-section of the root canal, streamlined, vector, and wall shear stress.

RESULTS

Laboratory analysis of EDTA 18% solution showed a density of 1.08 g/cm^3, viscosity of 0.178 cps, and a pH value of 7.80. The results of laboratory calculations for the $Ca(OH)_2$ medicament with a ratio of 1:1 using an aquadest vehicle showed a density of 1.34 g/cm^3, viscosity of 977 cps, and pH value of 12.73 (Table 1).

Table 1. Properties analysis results of EDTA 18% and $Ca(OH)_2$ fluids

Fluids	Value		
	Density (g/cm^3)	Viscosity (cps)	pH
EDTA 18%	1.08	0.19	7.80
$Ca(OH)_2$	1.34	977	12.73

The CAD geometric model of the root canal (Figure 3) and the CAD irrigation needle design results using the SpaceClaim© software from the MICRO-CT scanning result were included in the data processing. The code of Ansys Fluent 17.1 (Ansys Inc, USA) was used to prepare and resolve problems and analyse the results of this study. The Navier-Stokes equation that describes incompressible, three-dimensional, and time-based fluid flow, was solved by the iterative solver. The mathematical solution method used was a finite volume approach.

Figure 3 shows the direction of fluid flow in vector form. Fluid flow is seen in the form of arrows with colours according to the velocity of flow in the area. Laminar flow is seen in this research model. Low turbulence is formed in the irrigation needle lumen close to the inlet (side vent irrigation needle), while in the inlet (side vent irrigation needle) and the entire root canal did not show any turbulent phenomenon.

The highest velocity of irrigation flow was found in the lumen marked in red (19 ms^{-1}) when the direction of flow was seen in the form of arrows from the inlet to the outlet. Velocity decreased due to changes in the area in the inlet (side-vent irrigation needle). The maximum velocity in the root canal was seen around the inlet indicated by the green arrow (side-vent irrigation needle) which is around 9 ms^{-1}.

The arrows in the figure show the direction of flow that originates from the inlet towards the apical then curves to form a small clockwise vortex turned towards the outlet (root canal orifice) through the distal surface of the irrigation needle, so that the flow moves in the apical part of the irrigation needle tip to the channel apex roots show stagnant (dead zone) behaviour.

Figure 4 shows the root canal wall shear stress formed on the area facing the apical part of the inlet (side-vent irrigation needle). The highest wall shear stress is marked by a red area of 1.56 KPa seen in the area. This picture corresponds to the highest velocity of irrigation flow found in the area in the root canal.

The numerical results of CFD simulations are shown in Table 2. The highest velocity of EDTA 18% solution is found in the irrigation needle lumen of 19 ms^{-1}, wall shear stress of EDTA 18% solution to the root canal wall was maximum at 1.56 KPa.

Table 2. CFD simulation numeric results

Numeric parameters	Value
Maximum velocity of EDTA 18%	**19 ms^{-1}**
Wall shear stress of EDTA 18%	1.56 KPa

DISCUSSION

The development of research methods and models in the field of root canal irrigation has led to a better understanding of the efficiency and effectiveness of channel irrigation to improve the

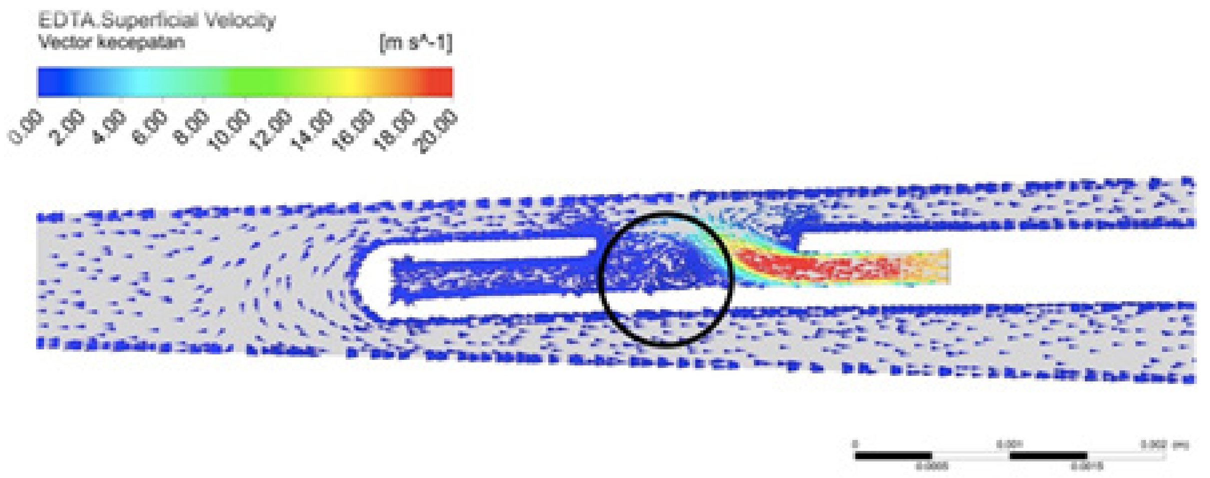

Figure 3. Vector simulation results show low turbulent values seen in areas marked with dark circles

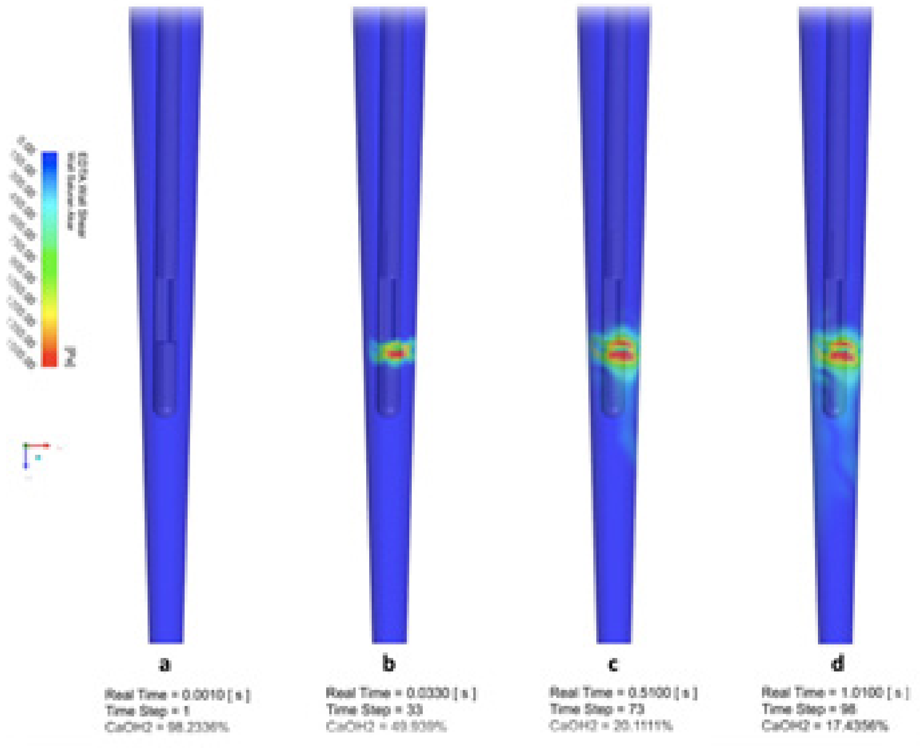

Figure 4. Wall shear stress contour simulation results

quality of endodontic treatments. Differences that occur between clinical conditions (in vivo) and laboratory conditions (in-vitro) observed, such as root canals in the oral cavity. This difference can be narrowed with the Computational Fluid Dynamics (CFD) method, which is a method and model that can help understand the dynamics of fluid movement in the root canal.

CFD analysis focuses on predicting the phenomenon of fluid flow movements (hydrodynamic phenomena). This reason makes researchers choose the CFD method because this method can see the movement of irrigation solutions in the root canal, which is a 3-dimensional area that is difficult to observe with experimental research.[9,13] CFD studies produce detailed (numerical) parameters about physical phenomena in root canals including the direction of flow vectors, contours of flow movements, streamline flow, wall shear stress of the root canal, and volume fraction between solution and medicament in root canals according to the time of the study.

Velocity and wall shear effectiveness of irrigation solutions in root canals were evaluated by CFD methods and experimental methods using the slow-motion recording. Detailed comparisons of the flow generated by CFD and slow-motion recordings were conducted to validate the results of CFD studies, so that CFD research is appropriate or close to the real situation with an error value of less than 10^{-4}.[8,10] CFD compatibility and experimental research were seen from fluid flow movements in cleaning $Ca(OH)_2$ in root canals. The results of the validation of this study indicate the conformity of CFD research with experimental research.

Inlet velocity generated in this study with a flow rate of 0.26 mLs^{-1}, which was 9 ms^{-1}. These results were by the results of previous studies by Li et al[17] on root canal irrigation with different irrigation needles using CFD analysis with the resulting inlet velocity of 8.6 ms^{1}. Boutsioukis et al[16] in their study also showed a velocity inlet of 8.6 ms^{-1}. Irrigation needle inlet elasticity is a significant factor in determining the movement of flow in the root canal.[17]

Irrigation using EDTA 18% in CFD studies and experimental showed good fluid movement in cleaning calcium hydroxide medicaments in root canals. The experimental results showed a significant cleansing of the medicament from the first 5 seconds of irrigation to 60 seconds by leaving the medicament at the bottom of the tip of the irrigation needle; then the cleaning effect went very slowly with a not too significant difference in results. This result is consistent with the study of Carl et al. in 2002 that EDTA irrigation solutions work well up to 60 seconds, which makes it ideal for use as root canal irrigation solutions in clinical use.

The cleaning of calcium hydroxide medicaments in the root canal by irrigation of EDTA 18% solution using 30G side vent irrigation needles in this study was carried out up to 1-second simulation which requires 6 hours of running time. The simulation results of CFD for 1 second showed a reduction in the amount of calcium hydroxide medicament up to 14.9% from the initial amount. The initial number of medicaments in the root canal was 19.72 mg, while the final number during irrigation for 1 second was 4.84 mg.

The effects of irrigation primarily were the effect of flushing irrigation in the root canals, and partly dissolving irrigants and wall shears in the root canals due to fluid flow. Wall shear stress directly affects the quality and efficiency of cleaning the root canal walls. Wall shears are the main cause for removing layer smears and medicaments in the root canal walls. Li et al[17] mentioned that wall shear stress depends on the flow rate of the irrigant. Increased flow rate causes the wall shear stress to increase gradually. The geometry of the irrigation needle affects simultaneously.[17]

This study observed the contour of wall shear stress to analyse the shearing effect of the irrigant flow. The highest effect of the wall shear stress was seen on the side facing the inlet (side vent of the irrigation needle), which showed the best shearing effect in the area. This result was by the research of Li et al[17] in the research on the effectiveness of various forms of numerical irrigation needles, stating that the shape and size of irrigation needles can determine the depth of the flow of irrigation, fluid agitation, and canal wall shearing effect.[17]

The results of our research showed that EDTA 18% solution gives a significant picture of the removal of calcium hydroxide medicaments in root canals. The use of irrigation needle forms can be modified to increase the effect of irrigation; further research is needed on the geometry, number, and position of irrigation needle vents to obtain better irrigation efficiency.

CONCLUSION

Velocity and wall shear stress of EDTA 18% showed the results validation conformity between experimental and CFD, that the maximum velocity of EDTA 18% is 19 ms^{-1} and EDTA 18% wall shear stress is 1.56 KPa for calcium hydroxide removal observed from the CFD study.

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