

RESEARCH ARTICLE

Streamline characteristics using the computational fluid dynamic analysis in the flow of 18% EDTA irrigation solution to remove Ca(OH)₂

Anna Muryani*, Hendra Dian Adhita Dharsono*, Z. Zuleika*, Ing. Mochammad Agoes Moelyadi**, Diani Prisinda*

*Department of Operative Dentistry and Endodontic, Universitas Padjadjaran, Bandung, West Java, Indonesia

**Faculty of Mechanical and Aerospace Engineering Bandung, Institut Teknologi Bandung, Bandung, West Java, Indonesia

*Jl Sekeloa Selatan No 1, Bandung, West Java, Indonesia; e-mail: anna.muryani@fkg.unpad.ac.idSubmitted: 27th November 2017; Revised: 6th March 2018; Accepted: 18th July 2018**ABSTRACT**

The remaining calcium hydroxide (Ca(OH)₂) medicaments in the root canal wall can block the penetration of filling medicaments to the dentine tubule and cause the failure in the root canal treatment. One of the ways in cleaning the root canal wall from the remains of Ca(OH)₂ is by using 18% Ethylene Diamine Tetra Acetic Acid (EDTA) irrigation solution. The cleanliness of the root canal can be examined using the Computational Fluid Dynamics (CFD) analysis. The aim of this research was to see the description of the cleanliness of the root canal wall from the Ca(OH)₂ medicament with 18% EDTA irrigation by means of CFD analysis. This is a descriptive-explorative research. Having been validated with the experimental research using test specimen in the form of block resin made in accordance with the characteristics of root canal, the description of the cleanliness of the root canal wall from the Ca(OH)₂ medicament with the 18% EDTA irrigation was analyzed using CFD method. The irrigation needle used was the side-vented type with the position of 3 mm from the tooth apical. The results of the research showed the conformity between the result of experimental research and CFD research. One of the results of this research was the characteristics of streamline of 18% EDTA in the root canal showing a unique behavior due to the characteristics of the form of side vent irrigation needle. The irrigation flow in the coronal area of the inlet (side vent irrigation needle) showed a low velocity causing the more fluid flowing out from the inlet went to apical rather to the outlet (root canal orifice). In conclusion, this research showed that 18% EDTA solution indicated the conformity of validation results between experimental research and CFD research in the frames of 5, 10, 15, and 20 secs observed from experimental research with the of frame 0,010, 0,099, 0,150 and 0,410 secs as observed from CFD research.

Keywords: Calcium hydroxide (Ca(OH)₂); computational fluid dynamics; EDTA; streamline; 18%

INTRODUCTION

The main aim of root canal treatment is to remove the microorganism in the root canal and to create a disadvantageous environment for the remaining microorganisms to survive.¹ Ca(OH)₂ possesses a good antimicrobial activity, and it is able to neutralize the bacterial endotoxin, stimulate the improvement process in the periapical tissues and is used to stimulate the root formation and hard tissues defence in the condition of root and tooth resorption with an incomplete root closure.²

Ca(OH)₂ medicament must be removed from the root canal wall prior to the filling action to prevent any *interference* between the filling materials and the root canal wall. Ca(OH)₂ medicament can

cause the block of dentin tubule of root canal making the medicament unpenetrated into tubule.^{2,3} The Ca(OH)₂ medicament remaining in the root canal wall can disturb the adhesive properties of filling materials towards the root canal wall and, in long term, it can lead to the failure of root canal treatment.⁴

The root canal wall cleanliness from the remains of Ca(OH)₂ is conducted by dissolving Ca(OH)₂ with an irrigation solution possessing the chelating properties in the root canal.⁵ 18% EDTA solution refers to a solution that functions as a chelating agent in which one of its usages is as an irrigation solution in the end of root canal treatment. This irrigation solution is also used as a lubricant

in the root canal and irrigation solution for cleaning the debris and inorganic smear layers after the root canal preparation. Research conducted by Perez-Heredia et al. (2008) informed that 15% EDTA solution was able to bind Ca^{2+} ions from dentin - better than other chelating agents.⁶

Many methods and models have been developed to study the root canal irrigation system; two of which have been done through experimental and computational methods. Computational Fluid Dynamics (CFD) is an analytical method for learning the way to predict the fluid flow, heat transfer, chemical reactions, and other flow phenomena by solving some mathematical equations (mathematical models).⁷⁻¹⁵

Research by Boutsoukis et al. (2009) began to introduce CFD model as an approach to evaluate the irrigation flow in root canal.¹⁶ An in-depth understanding of fluid flow characteristics is found difficult to be obtained using an experimental approach, but it can be easily by means of the CFD approach.¹¹ The CFD application has recently been widely used in dentistry in studying irrigation system on root canal treatment.¹⁴ Based on the information above, this study aims to describe the streamline characteristics using CFD analysis on the flow of 18% EDTA irrigation solution to remove $\text{Ca}(\text{OH})_2$.

MATERIALS AND METHODS

The preparation of research started by making the tested specimens for experimental research. Here, the tested specimens were in the form of 1 block resin of customized single root canal with geometric characteristics following the study of Boutsoukis C, et al. (2010) (Figure 1).¹⁶

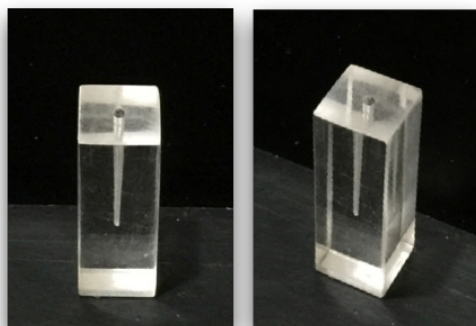


Figure 1. Block resin of customized root canal.¹⁷

This block resin was made through the phase of analysis on the form of frustum cone shaped canal geometry in which the root canal was 18 mm in length, 1.57 mm in orifice diameter, 0.45 mm in apical diameter and 6.2 % of taper (Figure 2).¹⁶

The application of $\text{Ca}(\text{OH})_2$ paste in the block resin of root canals was customized. The irrigation solution 18% EDTA used a side vent 30G irrigation needle in which the length of needle was reduced by 3 mm from the length of root canal for 19 seconds using a syringe pump with a flow rate of 0.26 mL/s. The process stage No. 3 was recorded using the Camcorder Full HD Super Slow Motion NXCAM (Sony NEX-FS700R) with the 105mm f/2.8 Macro lens (Sigma EX DG) with the help of the 5400K Super Bright LED Panel (NanGuang CN-2000). The observation of $\text{Ca}(\text{OH})_2$ paste in root canals was carried out based upon the pattern of particle movement in the root canal for 19 seconds.

The research preparation on CFD refers to the reconstruction phase of the geometry form of the first stage in the form of reconstruction of the root canal geometry by forming a geometric model of the root canal CAD following the size formed using SpaceClaim Software (Figure 3). This size was consistent with test specimens of root canal used in experimental research.

The reconstruction of the geometric form in the second stage refers to the analysis of the geometric form of the 30G side vent irrigation needle (*Prorinse Dentsply*) obtained from the results of *scanning micro computed tomography* (Micro-CT). Irrigation needles were arranged on plasticine with the tip of the 20 mm needle facing upwards and Micro-CT was conducted for 3 hours. The scanning results

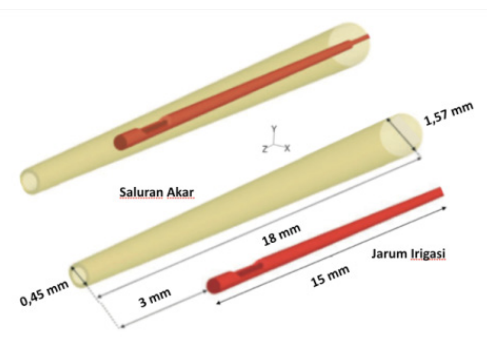


Figure 2. The design of shape and size of root canal test specimen.¹⁷

were reconstructed in the 3D form and the scanning results were verified with 0.30 mm of the external Dext needle, as informed in literature,¹⁷ and was formed into CAD using Spaceclaim Software. The needle length was adjusted to the simulated root canal length reduced by 3 mm (i.e. 15 mm). Irrigation needles would be placed at a distance of 3 mm from the apical end, positioned stable in the middle of the root canal (Figure 4).

The next step was the formation of mesh and domains of the flow, i.e. the surface of the inlet, outlet, and root canal wall constructed by using Pre-processor CFD Ansys Meshing Software's 17.1. The mesh formation consisted of pre-processing, processing and post-processing stages. The mesh construction used was in the form of 1,319,743 unstructured tetrahedrals arranged in the domain. The fluid flew into the simulated domain through the inlet (sidevent irrigation needle) and flew out through the outlet (root canal orifice) due to the provision of atmospheric pressure at the outlet.

The pre-processing phase started with the transfer of the CAD form of the root canal geometry model and the irrigation needle. Subsequently, the computational domain was formed in the root canal geometry model. The formation of mesh model occurred on the outer surface and volume in root canals and irrigation needles. Evaluation and improvement of mesh quality. Output: mesh, surface boundary, and terming.

The processing phase started by inserting (input) mesh with data of the chemical structure name of 18% EDTA fluid and $\text{Ca}(\text{OH})_2$, the input of the physical and chemical properties of fluid (density, viscosity, and pH), and the result of a chemical reaction to $\text{Ca}(\text{OH})_2$. It also included the determination of fluid flow equation models and physical models, numerical parameters, and numerical schemes. It was then continued with the analysis on 18% EDTA solution and root canal paste fully filled with $\text{Ca}(\text{OH})_2$ medicament and the needle fully filled with an irrigated solution. The impact of gravitation was inserted in the simulation as the potential energy occurred in the flow. The laboratory analysis was carried out to obtain density, viscosity, and pH values from 18% EDTA

solution, and paste $\text{Ca}(\text{OH})_2$. Fluid density was calculated using a picnometer, while fluid viscosity was calculated using the falling sphere viscometer. The CFD program was run (running the program) and the growth of errors was monitored. The results were then simulated and an the animation of the EDTA 18% irrigation process was made towards $\text{Ca}(\text{OH})_2$ in root canal using Ansys-Fluent Software.

The post-processing stage was conducted once obtaining animation in the form of the display of domain and mesh geometry. The flow pattern (streamlined and vector), speed contours, pressure contours, 2D image dimensions, and 3D animated videos were then analysed. Subsequently, an observation on output and velocity calculation (contours, vectors, and streamlined), wall shear stress, volume fraction of $\text{Ca}(\text{OH})_2$ medicaments and 18% EDTA solution and validation of the results of CFD research on experimental research were done. The calculation of CFD simulation was carried out 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. The volume and velocity fractions were monitored every timestep to ensure an adequate convergence. Computing was done using the computer of *Intel Xeon Processor 12 Core @ 2.00 GHz 128GB DDR3 ECC RAM 64bit* Operating System. The flow field was calculated to see the flow patterns, velocity magnitude, wall shear stress, and fluid volume fraction. *Lagrangian particle tracking* was also carried out at this stage. Tracking was done on the path of massless particles in the flow domain from the inlet to the outlet.

The results of the 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 PPDGS Dental Conservation Clinic of the Faculty of Dentistry, University of Padjadjaran, Computer Laboratory of RSGM FKG Padjadjaran University, Physics Laboratory of Institut Teknologi Bandung, Pharmaceutic Laboratory of the Institut Teknologi Bandung, and Aerogasics Laboratory and CFD of the Faculty of Mechanical Engineering and Aerospace Institut Teknologi Bandung. The data

analysis of experimental validation and CFD results were conducted using graphic data analysis.

RESULTS

Experimental research was carried out using customized block resin specimens (Figure 1). Eighteen percent EDTA solution was injected into the root canal containing $\text{Ca}(\text{OH})_2$ medicament using a 30 G 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 with the help of a 105 mm macro lens and a 5400K super bright LED panel. The results of the research were validated with the results of CFD research in the form of volume fraction of fluid movement patterns in the root canal wall. The research results of the CFD observed in this research showed the volume fraction in the cross section of the root canal, streamlined, vector, and wall shear stress.

The laboratory analysis of 18% EDTA solution had a density of 1.08 g/cm^3 , viscosity of 0.178 cps, and pH of 7.80. The results of laboratory calculations on the of $\text{Ca}(\text{OH})_2$ medicament with a ratio of 1:1 used a distillation water vehicle including the density of 1.34 g/cm^3 , viscosity of 977 cps, and pH 12.73 (Table 1).

This research is included in a research with the “*Multispecies*” stream. Multispecies describes the use of fluids with different types, namely 18% EDTA solution and $\text{Ca}(\text{OH})_2$ paste in the root canal. The resulted data included a CAD design of the geometric root canal model (Figure 3) as well as the results of the CAD irrigation needle design

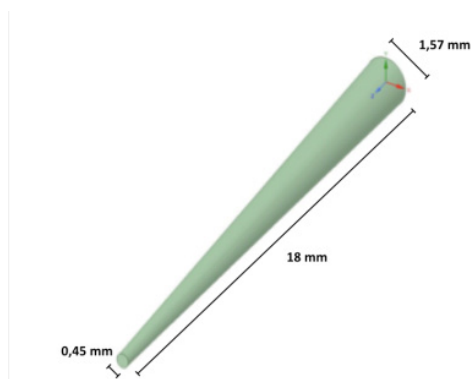


Figure 3. Design of CAD of geometric root canal model

using the spaceclaim software from the MICRO-CT scanning results included in processing data. Ansys Fluent 17.1 CFD Code (Ansys Inc, USA) was used to prepare and solve problems and analyze the results of this study. The Navier-Stokes equation describing 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 7 shows a streamline of 18% EDTA irrigation solution in the root canal. The streamline of 18% EDTA irrigation solution showed a unique behavior due to the characteristics of the side vent irrigation needle. The irrigation flow in the coronal area of the inlet (side vent irrigation needle) showed low velocity leading the flow of fluid when exiting from the inlet mostly went towards the apical rather than towards the outlet (root canal orifice).

Figure 7 A-C show a streamline flow of 4 frames of time based upon the initial entry entering through the needle inlets – a condition when fluid volume fraction reached 50%, and one third apical area began to form the dead zones. The analysis on the streamline velocity of irrigation in the z component direction of the cross section of the long root canal axis (z axis) showed the depth of the movement of the irrigation flow. The results of the analysis showed that irrigation at 4 frames of that time could not reach the distance to the root canal apex beyond the distance of 1–1.5 mm from the apical end of the irrigation needle.

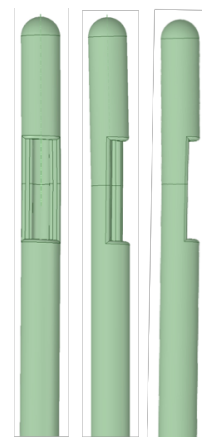


Figure 4. The results of CAD design of Irrigation Needle Using Space claim Software from the result of Micro-CT scanning

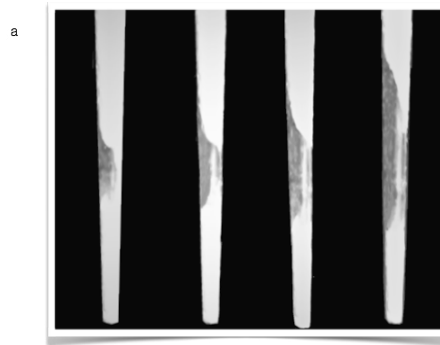


Figure 5. The image of the pattern in the movement of 18% EDTA irrigation solution to the Ca(OH)_2 medicament for 5, 10, 15, and 20 seconds.

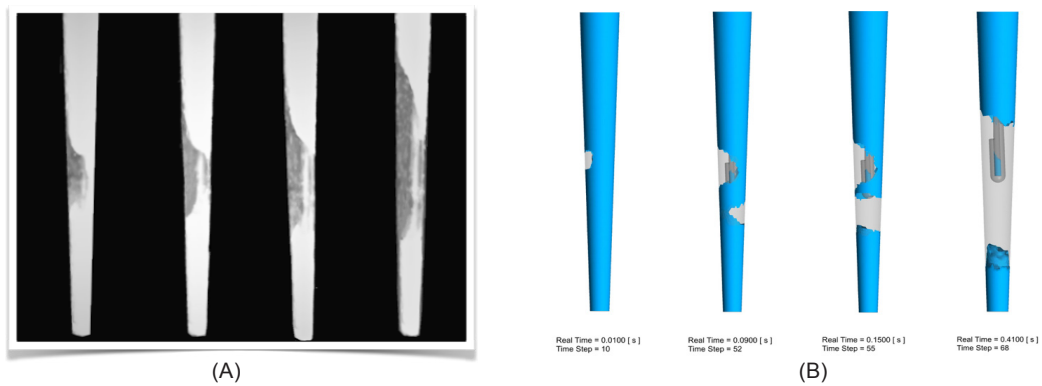


Figure 6. Validation between the pattern of the flow movement in (A) experimental research and (B) CFD research

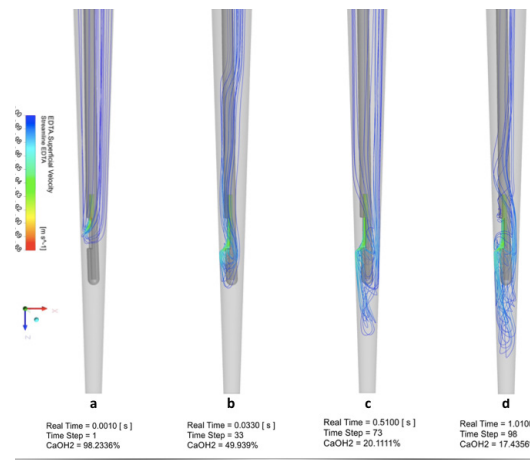


Figure 7. Result of simulation on the streamline in the time frame of (a) 0.001 secs; (b) 0.033 secs; (c) 0.510 secs and (d) 1.010 secs

Table 1. The results of the analysis on the properties of 18% EDTA fluid and Ca(OH)_2

Name Solution	of	Values		
		Density (g/ cm^3)	Viscosity (cps)	pH
18%EDTA		1.08	0,19	7.80
Ca(OH)_2		1.34	977	12.73

DISCUSSION

The development of science and technology in the endodontics field has been influenced by method and model of research in which the clinical trials and laboratory research complement to each other purposely to improve the quality of endodontic treatment. The difference between the two is difficult

to be controlled between clinical conditions (*in vivo*) such as root canals in the oral cavity and laboratory conditions (*in vitro*). The difference between these methods can be narrowed by the research on physical realism. The Computational Fluid Dynamics (CFD) method refers to a method and model in endodontic research that can help to understand the dynamics of fluid movement in the root canal. Commonly, fluid flow is studied through one of the following three ways: experimental fluid dynamics; theoretical fluid dynamics; and computational fluid dynamics. CFD refers to a science that focuses on predicting the phenomenon of fluid flow movements (*hydrodynamic phenomenon*). The above reason has led the researchers to select the CFD method considering that this method is able to see the movement of irrigation solution in the root canal that is a 3-dimensional area that is difficult to be observed with experimental research.^{8,11} Research on CFDs has produced the detailed (numerical) and comprehensive parameters regarding the physical phenomenon in the root canal including the direction of flow vectors, contours of flow movements, streamline flow, wall shear root canal stress, and volume fraction between solution and medicament in root canal based upon the period of time of the research.

CFD validation must be done with the results of experimental research from the model as studied by Li.P et al. (2013) and Gao et al. (2009) in their research using high-speed camera techniques. This study used a high-speed Super Slow Motion (Sony NEX-FS700R) 960 frame/second camcorder for 19 seconds with the help of a 105-mm macro lens and a 5400K super bright LED panel.^{12,13}

In this research, the description of the flow of irrigation solution in the root canal was evaluated by two methods, namely the CFD method and the experimental method using slow motion recording. The detailed comparison of the flow generated by CFD and slow motion recording was conducted for the validation of the results of CFD study, so that CFD research was in line with or approached with real condition with an error value less than 10^{-4} .

The suitability of CFD and experimental research can be seen from the pattern of fluid flow

movement in cleaning Ca(OH)_2 in the root canals. The result of the validation from this study indicated the suitability of CFD research with the experimental research.

The time difference between experimental research and CFD research was probably due to the chemical reaction rate parameters between 18% EDTA solution and the Ca(OH)_2 medicament not included in the CFD research. Further research is suggested to include the reaction rate parameters so that the research time between experimental research and CFD research will be appropriate but in this study the time interval between experimental research and CFD research has shown a similar value, thus increasing the validity of CFD research on the experiment.

The streamline of irrigation solution illustrates the path of massless particles originating coming from the *inlet* of irrigation needle with color according to the velocity quantity of the irrigation solution flow in the root canal. The description of irrigation solution streamline in this study showed a unique behavior due to the characteristics of the side vent irrigation needle shape. The description of movement of fluid flow showed the flow of irrigation material formed in the lumen of the needle before reaching the needle inlet, and then formed a jet stream that rubbed against the side facing the needle inlet due to impulsive changes in the flow area. The jet stream flew towards the tip of the needle and rotated to follow the angle shape of the tip of the irrigation needle. This phenomenon is known as *Moffat's corner vortices*, and then flew through the back of the inlet (side vent irrigation needle) to the outlet of the root canal orifice. The irrigation process removed bacteria, debris, biofilms, and medicaments in the root canal due to the rinsing effect of irrigation (irrigant flushing effect).^{12,15,16}

The apical tierce area is an important area for the success of endodontic treatment. This study resulted in ineffective hygiene in the area of the apical tierce area especially in the end of the root canal to 1–1.5 mm from the tip of the irrigation needle. These results were consistent with the study of Boutsoukis et al. (2009) that the movement of

irrigation solutions is very limited in the apical part of the root canal.¹⁷ The researcher stated that efforts to increase the inlet velocity can make the irrigation solution movement more efficiently, but this effect is limited to only 1– 1.5 mm of apical direction from the tip of the irrigation needle.^{8,17}

CONCLUSION

This research showed the conformity between the streamline characteristics in the 18% EDTA of irrigation solution flow to the removal of Ca(OH)₂ between experimental research and the CPD analysis with a pattern corresponding to the fluid flow at 5, 10, 15 and 20 seconds.

ACKNOWLEDGEMENT

Our gratitude is addressed to the Faculty of Dentistry, Padjadjaran University, Directorate of Research, Community Service and Innovation at Padjadjaran University, Center for Oral Biomaterial Studies, FKG UNPAD, for providing the financial support in the form of fundamental research grants UNPAD (RFU) and Department/Study Program of Dental Conservation FKG UNPAD, Faculty of Mechanical Engineering and Aerospace of ITB, Faculty of Pharmacy of ITB, and Faculty of Physics ITB that have helped this research enabling it to run smoothly and achieved the expected results.

REFERENCES

1. Athanassiadis B, Abbott PV, Walsh LJ. The use of calcium hydroxide, antibiotics and biocides as antimicrobial medicaments in endodontics. *Aust Dent J.* 2007; 52: S64–82.
2. De Faria-Júnior NB, Keine KC, Só MVR, Weckwerth PH, Guerreiro-Tanomaru JM, Kuga MC. Residues of calcium hydroxide-based intracanal medication associated with different vehicles: a scanning electron microscopy evaluation. *Microsc Res Tech.* 2012; 75(7): 898–902.
3. Calt S, Serper A. Dentinal tubule penetration of root canal sealers after root canal dressing with calcium hydroxide. *J Endod.* 1999; 25(6): 431–433.
4. Kim SK, Kim YO. Influence of calcium hydroxide intracanal medication on apical seal. *Int Endod J.* 2002; 35(7): 623–628.
5. Deepak BS, Sherin JC, Mallikarjun GK. Removal of intracanal antiseptic medication; a review. *UJMDS.* 2014; 02(03): 136–142.
6. Pe´Rez-Heredia CM, Ferrer-Luque MP, Gonza´Lez-Rodri´Guez FJM-P&, Gonza´Lez-Lo´Pez S. Decalcifying Effect of 15% EDTA, 15% Citric Acid, 5% Phosphoric Acid and 2.5% Sodium Hypochlorite on Root Canal Dentine. *Int Endod J.* 2008; 41(5): 418–423.
7. Van Der Sluis LWM, Wu MK, Wesselink PR. The evaluation of removal of calcium hydroxide paste from an artificial standardized groove in the apical root canal using different irrigation methodologies. *Int Endod J.* 2007; 40(1): 52–57.
8. Shen Y, Gao Y, Lin J, Ma J, Wang Z, Haapasalo M. Methods and models to study irrigation. *Endodontic Topics.* 2012; 27(1): 3–34.
9. Anderson Jr JD. *Computational fluid dynamics the basics with applications.* 1st ed. USA: McGraw-Hill; 1995, 574-576.
10. Basrani B. *Endodontic Irrigation-chemical disinfection of the root canal system.* 1st ed. Springer International Publishing: Switzerland; 2015. 45-116.
11. Boutsoukias C, Lambrianidis T, Kastrinakis E. Irrigant flow within a prepared root canal using various flow rates: a computational fluid dynamics study. *Int Endod J.* 2009; 42(2): 144–155.
12. Li P, Zhang D, Xie Y, Lan J. Numerical investigation of root canal irrigation adopting innovative needles with dimple and protrusion. *Acta Bioeng Biomech.* 2013; 15(1): 43–50.
13. Gao Y, Haapasalo M, Shen Y, Wu H, Li B, Ruse ND, et al. Development and validation of a three-dimensional computational fluid dynamics model of root canal irrigation. *J Endod.* 2009; 35(9): 1282–1287. doi:10.1016/J.Joen.2009.06.018
14. Tuakia F. *Dasar-Dasar CFD Menggunakan FLUENT.* Informatika, Bandung. 2008.

15. Zhang PL, Xie Y, Lan J. Numerical investigation of root canal irrigation adopting innovative needles with dimple and protrusion. *Acta Bioeng Biomech.* 2013; 15(1): 43-50.
16. Boutsoukis C, Verhaagen B, Versluis M, Kastrinakis E, Van Der Sluis LWM. Irrigant flow in the root canal: experimental validation of an unsteady computational fluid dynamics model using high-speed imaging. *Int Endod J.* 2010; 43(5): 393–403.
17. Boutsoukis C, Verhaagen B, Versluis M, Kastrinakis E, Wesselink PR, Van Der Sluis LWM. Evaluation of irrigant flow in the root canal using different needle types by an unsteady computational fluid dynamics model. *J Endod.* 2010; 36(5): 875–879.
doi: 10.1016/J.Joen.2009.12.026