

Put your best teeth forward:

A mass transfer study of Crest Whitestrips

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Executive Summary:

Crest Whitestrips are thin, liquid films adhered to a plastic exterior that can be applied directly to the tooth, enabling mass transfer of its active ingredient, hydrogen peroxide, to penetrate the tooth outer layer. The tooth outer layer consists of enamel and dentin. The goal of this study was to model the concentration of hydrogen peroxide as it moves through the gel tooth outer layer for a period of 30 minutes. GAMBIT was used to create a two-dimensional mesh modeling the three layers through which the hydrogen peroxide diffuses through: the gel, enamel and dentin. FIDAP was then used to model the process in which hydrogen peroxide moved through these three layers. A sensitivity analysis was performed varying the diffusion coefficients and reaction rate of hydrogen peroxide being used up. It was found that accurate values for all of these properties must be obtained in order to determine an accurate solution.

Introduction:

In the past, only the rich and famous were able to afford the luxury of a perfect white smile. Now, new products have enabled easy and affordable teeth whitening methods from the comforts of home. One of the leading teeth whitening products on the market today is Crest Whitestrips.

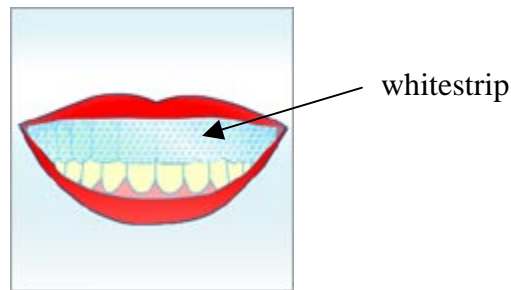


Figure 1: Teeth with white strip adhered

Crest Whitestrips are thin, liquid films adhered to a plastic exterior that can be applied directly to the tooth, enabling mass transfer of its active ingredients to penetrate the tooth outer layer. The strip device consists of a uniform amount of whitening gel and protects the gel from salivary interaction during the whitening process. The active ingredient Crest Whitestrips is hydrogen peroxide, which not only diffuses through the outer layers of the tooth but also reacts with organic material (stains) that it encounters. Crest Whitestrips are suggested to be left on for 30 minutes at a time, but how far is the hydrogen peroxide actually penetrating through the tooth?

There are two layers of the tooth that the hydrogen peroxide diffuses through: the enamel and the dentin (Fig _).



Figure 2: Layers of tooth.

Design Objectives:

The main objective of using whitening strips is to provide a safe and effective method that distributes the bleaching agent, hydrogen peroxide, through the teeth to react with, thus eliminating, the organic material that stain the teeth. The goal of this study was to model the concentration of the active ingredient, hydrogen peroxide, as it moves through the teeth. GAMBIT was used to create a two-dimensional mesh modeling the three layers through which the hydrogen peroxide diffuses through: the gel, enamel and dentin. FIDAP was then used to model the process in which hydrogen peroxide moved through these three layers.

Schematic:

In determining the geometry of the teeth treated with a Crest Whitestrip, we assumed that all the teeth being treated were equal in size to the incisor tooth. We modeled the tooth as a flat, finite plate with one-dimensional mass diffusion through the tooth (Schematic).

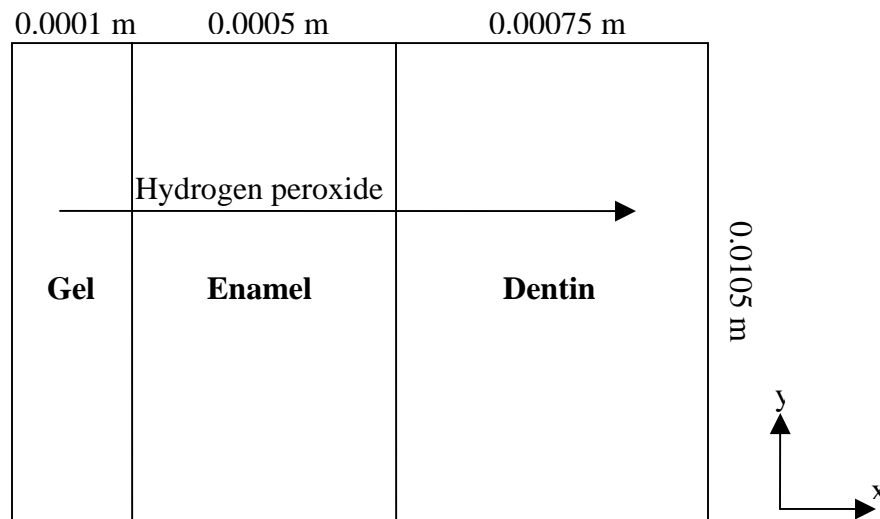


Figure 3: Schematic and dimensions of three layers (gel, enamel, and dentin) that hydrogen peroxide moves through.

Assumptions:

- (1) Tooth is flat, finite plate.
- (2) 1-dimensional mass diffusion through gel and tooth.
- (3) All teeth are equal in size to incisor tooth.
- (4) Properties of enamel and dentin are the same.

- (5) Diffusivity of tooth layers equal to that of bone.
- (6) Water and hydrogen peroxide are similar sized molecules.
- (7) Diffusion coefficient for hydrogen peroxide through enamel and dentin is equal to diffusion coefficient of water through bone.
- (8) Gel is made solely of glycerin.
- (9) Reaction rate is very small ($1/10^9$ times the organic material (tooth stain) reaction rate).
- (10) Application of white strip is for 30 minutes (1800 seconds).
- (11) Constant properties.
- (12) Isothermal.

Results and Discussion:

(I) Qualitative Description

As hydrogen peroxide, the active ingredient in the white strip, diffuses through the gel and the enamel and the dentin of the tooth, it is also used up in a chemical reaction. The hydrogen peroxide reacts with the organic material on and in the teeth that are the components of teeth stains.

We found diffusivity and reaction rates for the hydrogen peroxide in teeth and the gel from literature research (see Appendix A). In order to find these values, we had to assume that the diffusivity was the same in the dentin and enamel layers of the teeth and that these layers had the same diffusivity as bone. We chose to convert our time values from seconds to a non-dimensional value because our model was not working correctly with an end time of 1800 seconds. In order to determine the non-dimensional values, we scaled our total thickness of the geometry (including gel, enamel, and dentin) to 1.0. We then used the formula $D_0 \cdot t / L^2$ to find our non-dimensional end time. Figures 4A and 4B show the diffusion of the hydrogen peroxide through the whitening strip gel, the enamel, and the dentin.

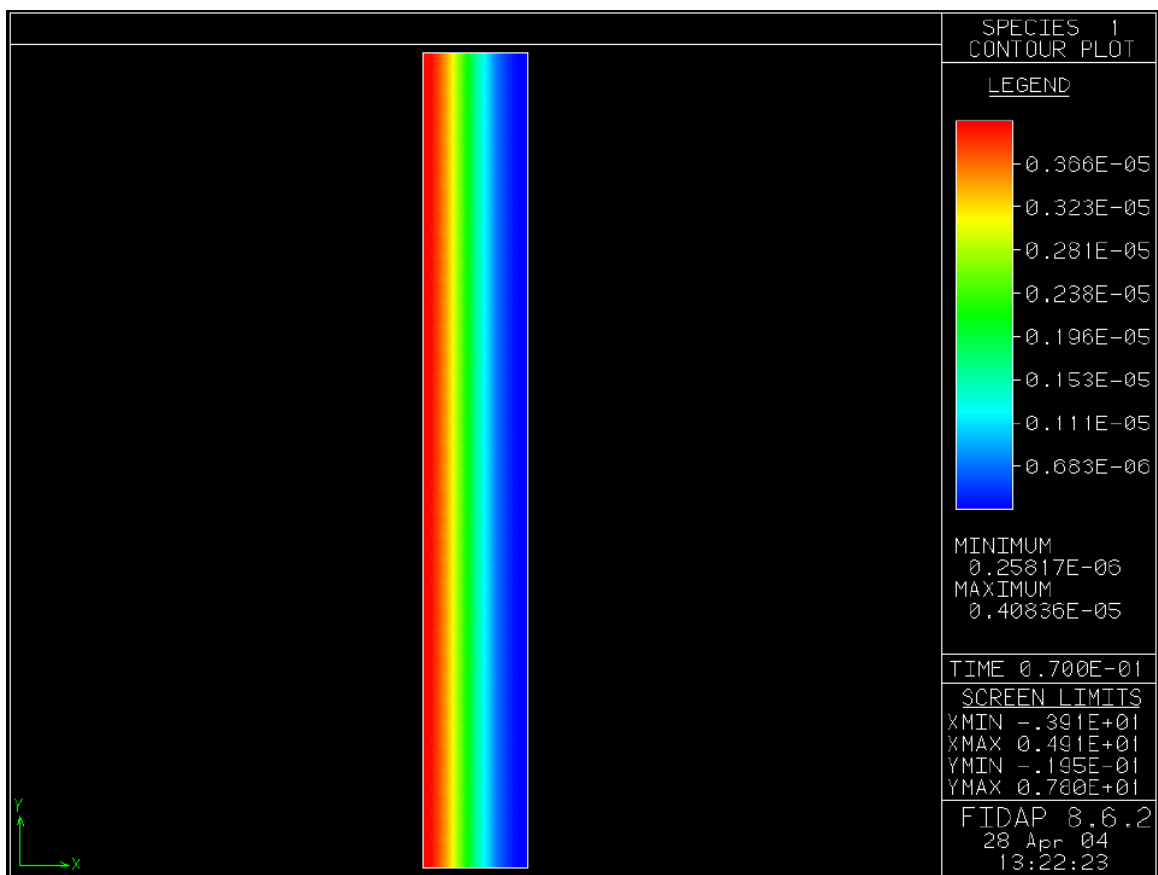


Figure 4A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). The initial concentration of hydrogen peroxide in the gel was 2.8×10^{-5} g/L.

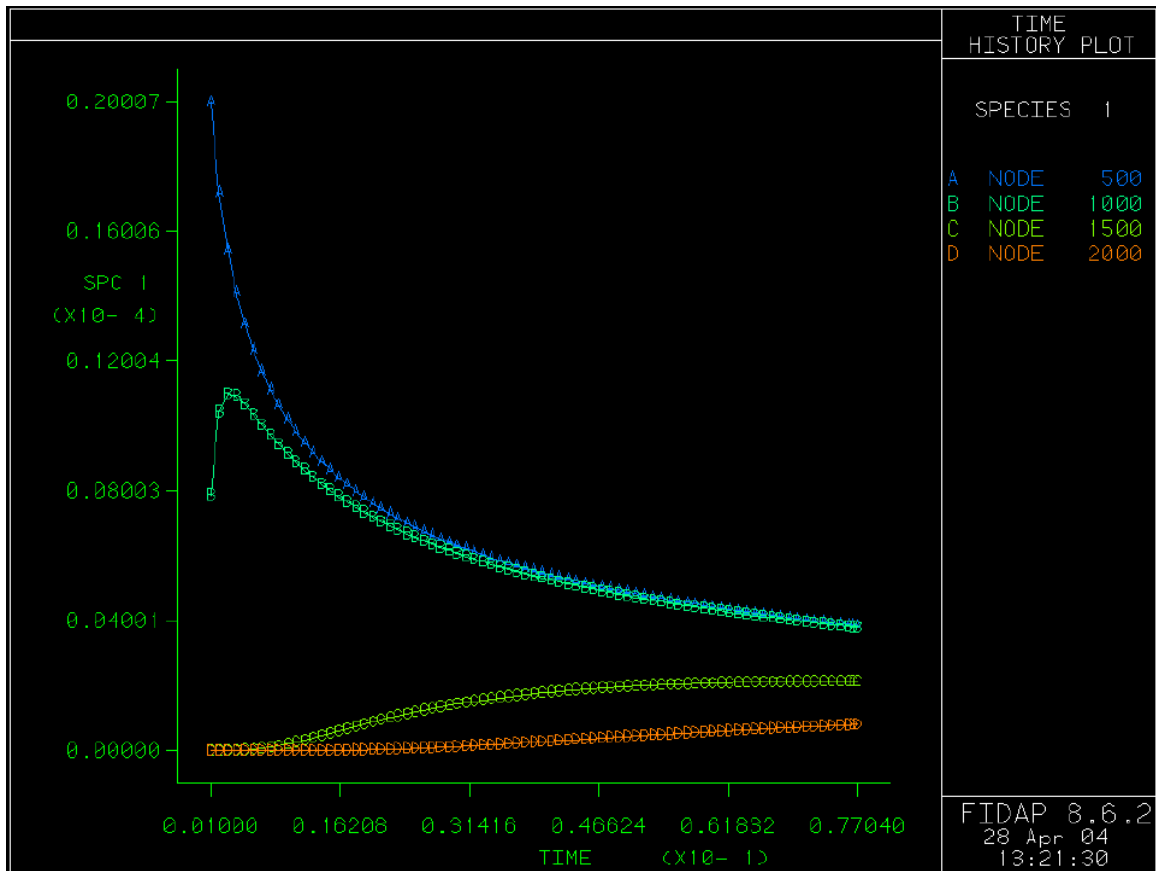


Figure 4B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin.

Figure 5 effectively displays how the concentration of hydrogen peroxide in the enamel and the dentin layers of the teeth increases with time while the concentration decreases with time in the gel and on top of the enamel.

(II) Sensitivity Analysis

In order to determine the effect of various properties on the solution, the values of diffusivity in both the enamel and the dentin and rate of the hydrogen peroxide reaction were varied from the accepted values.

Figures 5 through 7 show the model of diffusion of hydrogen peroxide through the gel and tooth layers as the diffusivity value of the dentin is varied, while the diffusivity values in the gel and enamel and all the other properties were kept constant. The diffusivity value was varied from one-half its original value to twelve times the original value. We chose to include the two extreme cases as well as the original in this report.

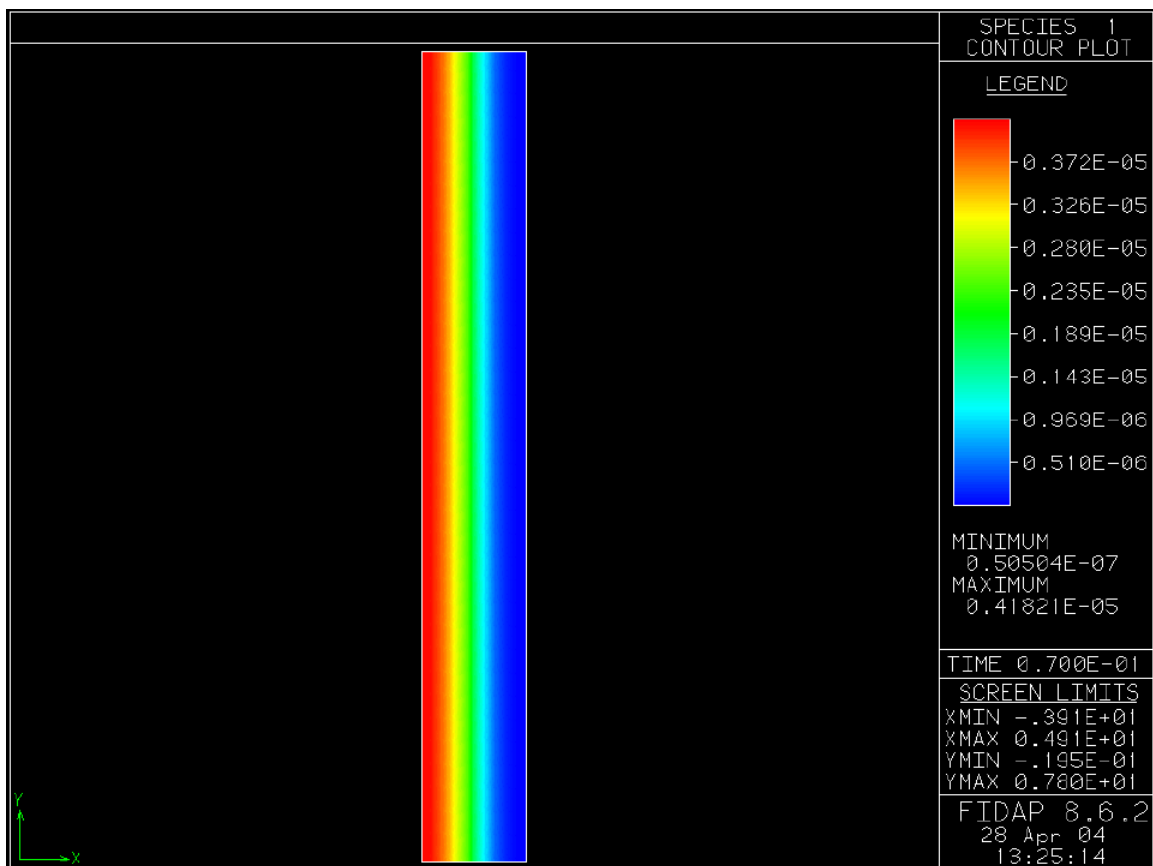


Figure 5A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Diffusivity of dentin = $\frac{1}{2}$ original value = $3.9 \cdot 10^{-11} \text{ m}^2/\text{s}$.

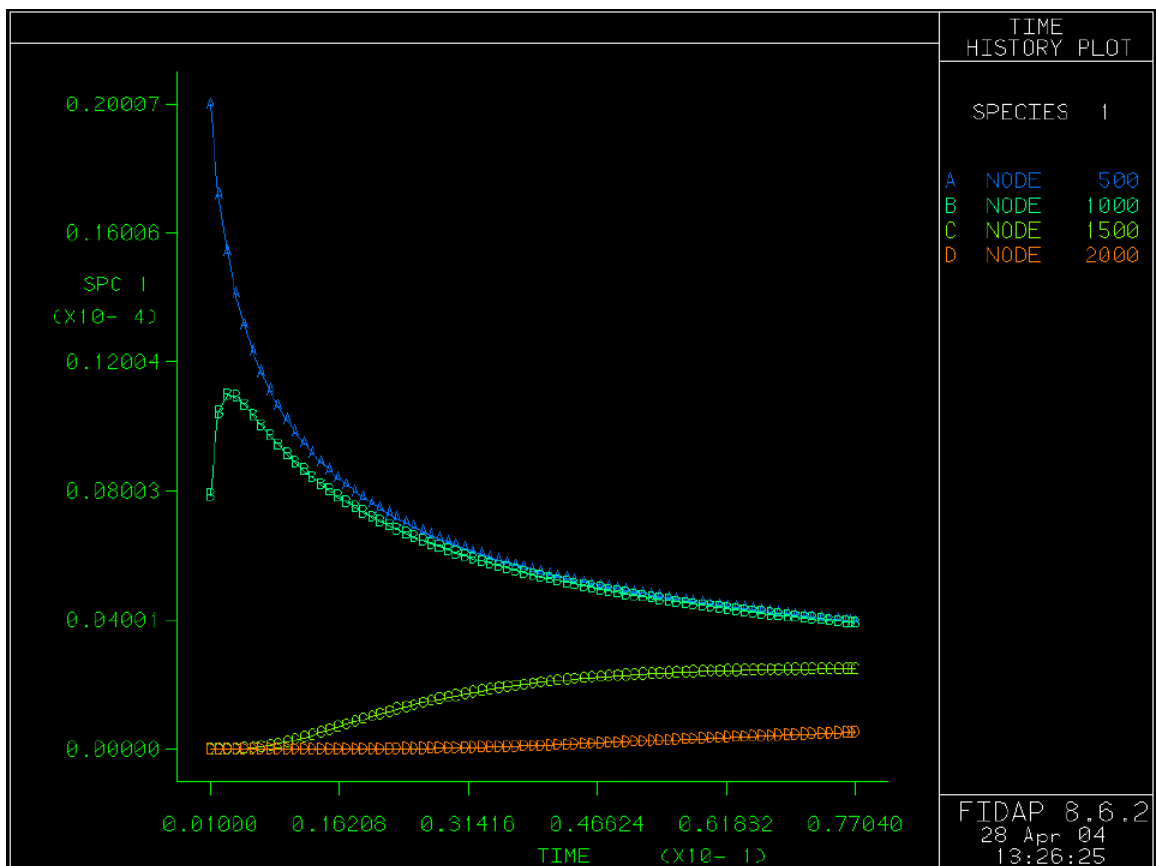


Figure 5B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Dentin diffusivity = $\frac{1}{2}$ original value = $3.9 \times 10^{-11} \text{ m}^2/\text{s}$.

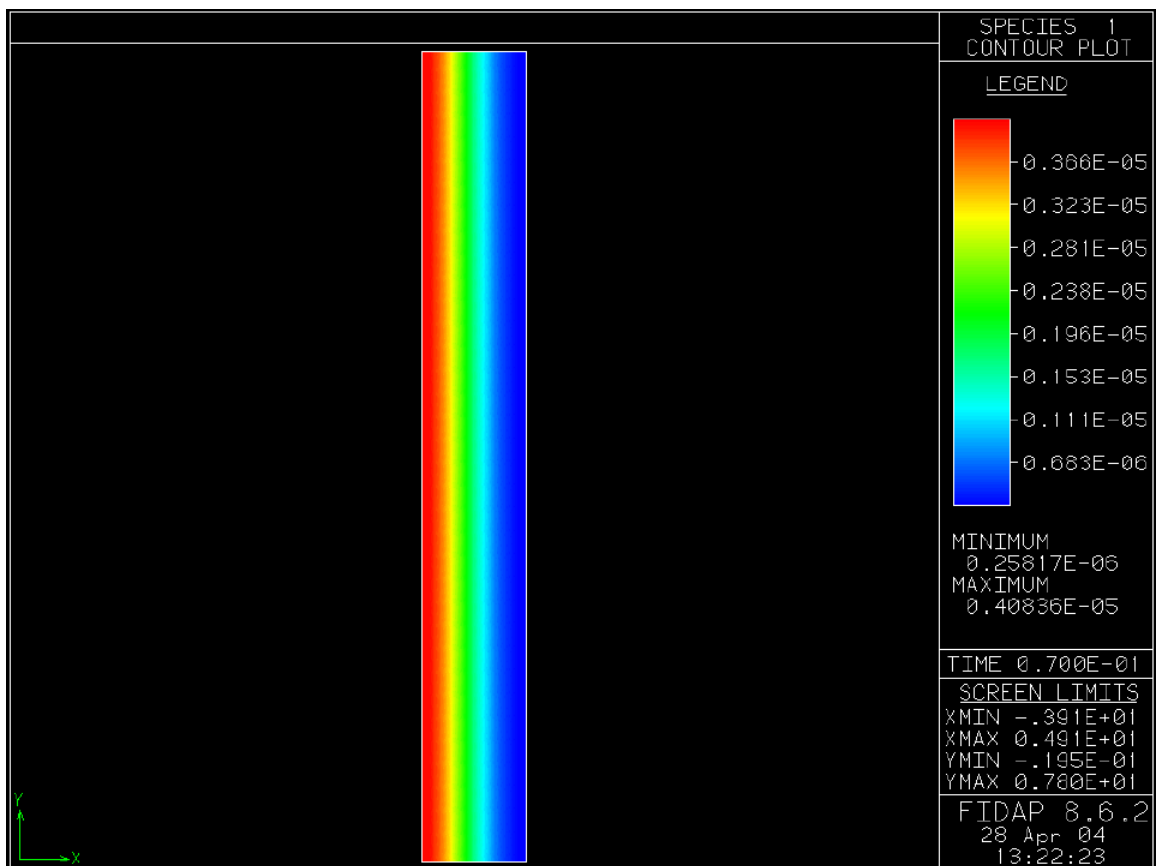


Figure 6A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Diffusivity of dentin = original value = $7.8 \times 10^{-11} \text{ m}^2/\text{s}$.

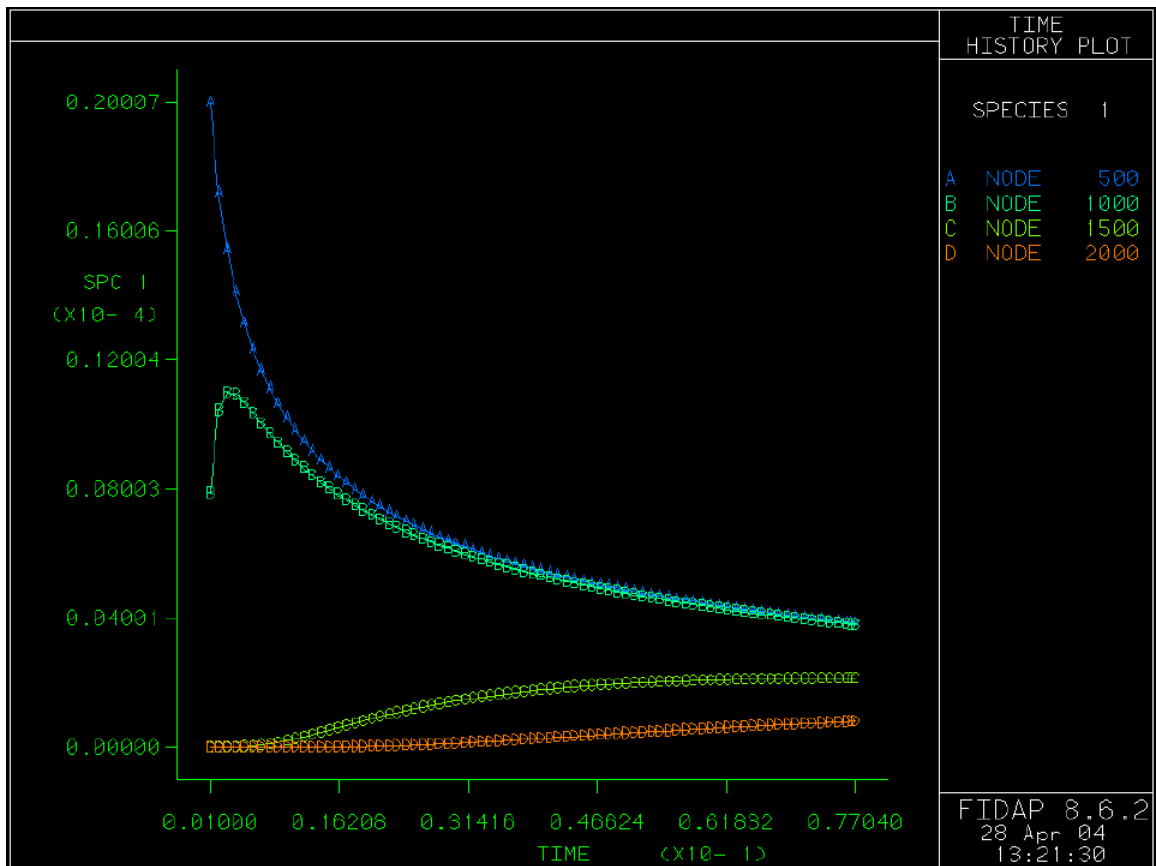


Figure 6B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Dentin diffusivity = original value = $7.8 \times 10^{-11} \text{ m}^2/\text{s}$.

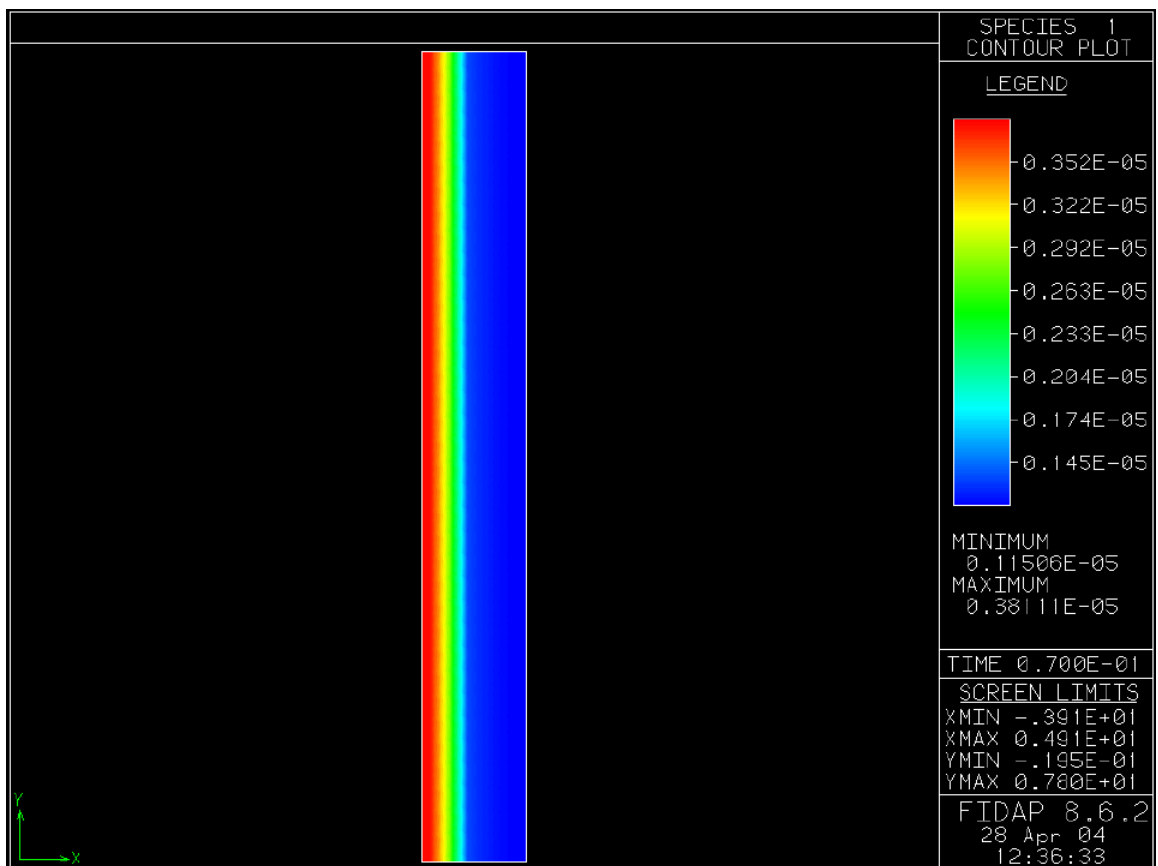


Figure 7A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Diffusivity of dentin = 12* original value = $9.4 \times 10^{-10} \text{ m}^2/\text{s}$.

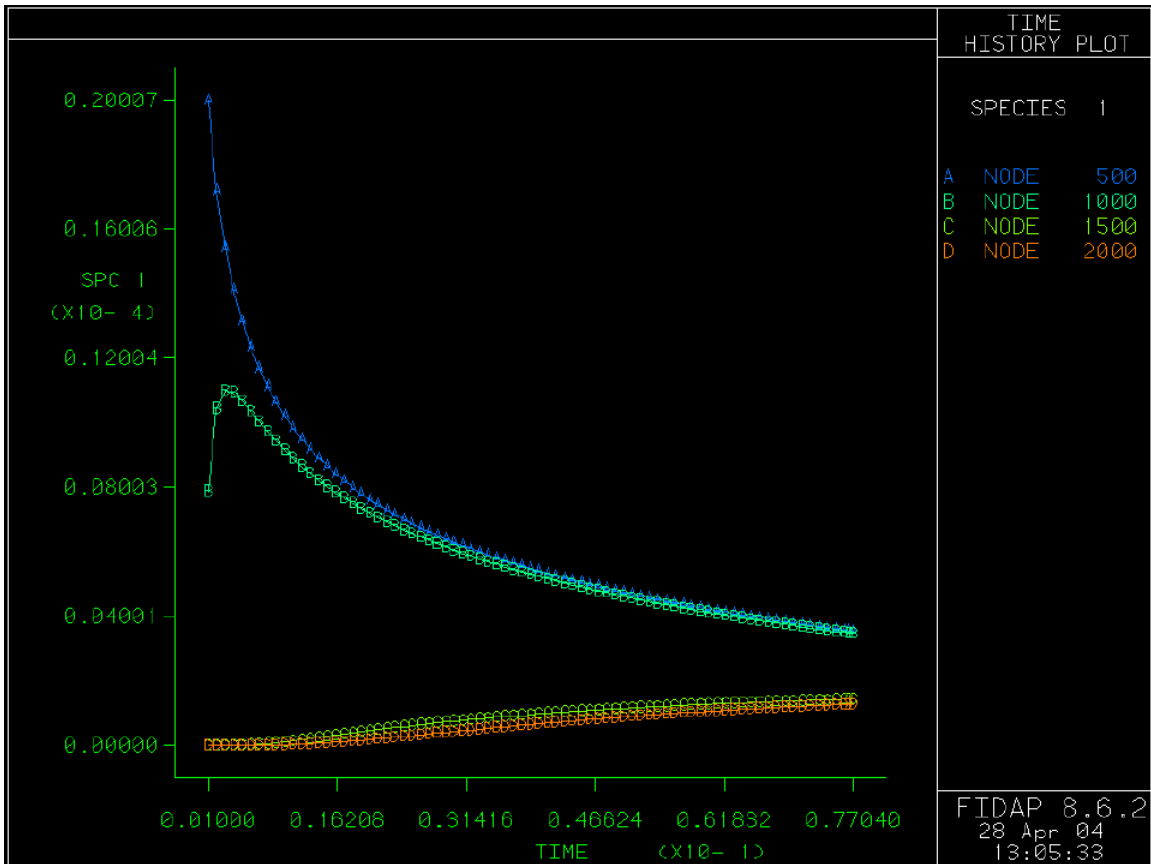


Figure 7B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Dentin diffusivity = 12* original value = $9.4 \times 10^{-10} \text{ m}^2/\text{s}$.

From these figures, there are some trends to be noted. As the diffusivity of the dentin is increased, the concentration of hydrogen peroxide in the enamel decreases and eventually becomes approximately equal to the concentration in dentin (seen in Figure 7B). This occurs because as the dentin diffusivity increases, the resistance to hydrogen peroxide diffusion decreases, making it very easy for the peroxide to move through the dentin layer. Similarly, Figure 5B shows that as the diffusivity of the dentin is decreased, the concentration of hydrogen peroxide increases while that in the dentin decreases when compared to Figure 6B (the original dentin diffusivity). In reality, this case where the dentin diffusivity is less than that of the enamel is not possible. Although we assumed that the enamel and dentin have the same diffusivity coefficient because we couldn't find values for each layer, the enamel is actually harder than the dentin and therefore its diffusivity is actually less than that of dentin.

Figures 8 through 10 display the diffusion of hydrogen peroxide through the gel and tooth layers as the diffusivity value of the enamel is varied, while the diffusivity values in the gel and dentin as well as all other properties were kept constant. The diffusivity value was varied from one-fourth its original value to five times the original value. We chose to include the two extreme cases as well as the original in this report.

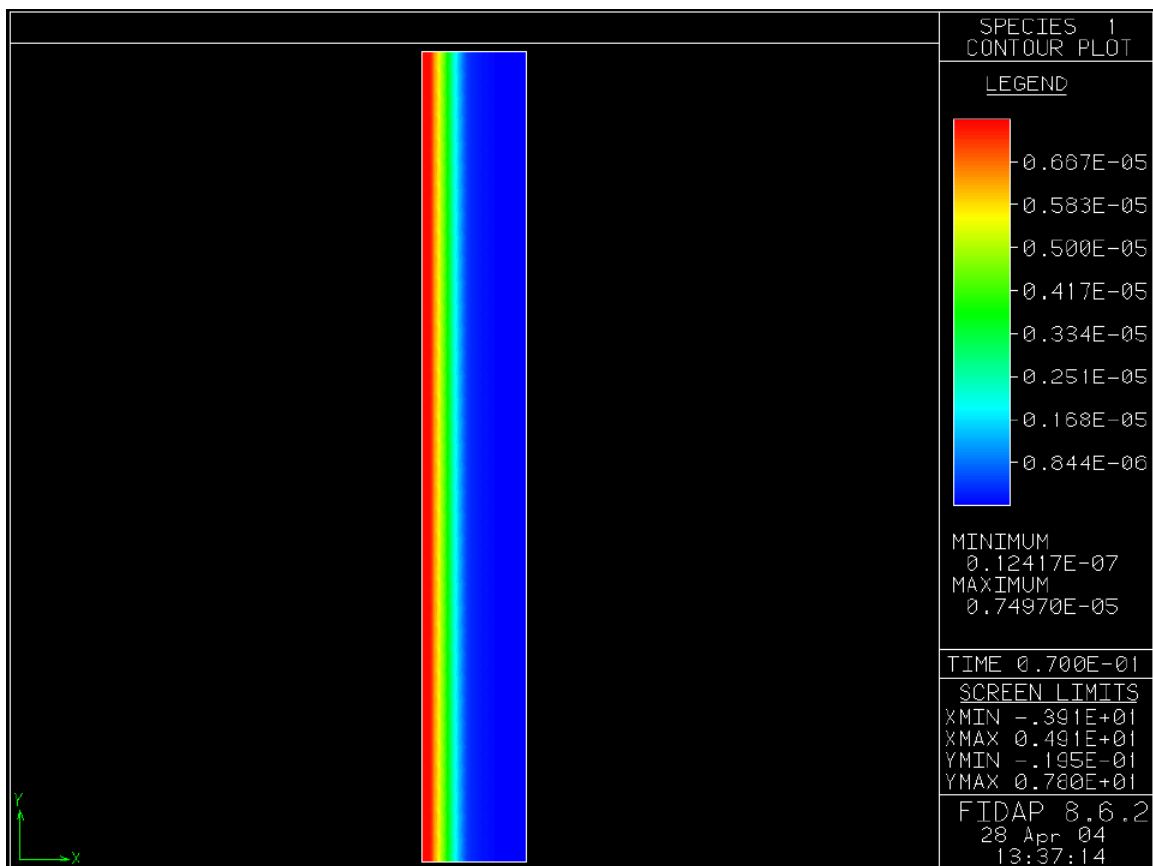


Figure 8A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Diffusivity of enamel = $\frac{1}{4}$ * original value = $1.95 \cdot 10^{-11} \text{ m}^2/\text{s}$.

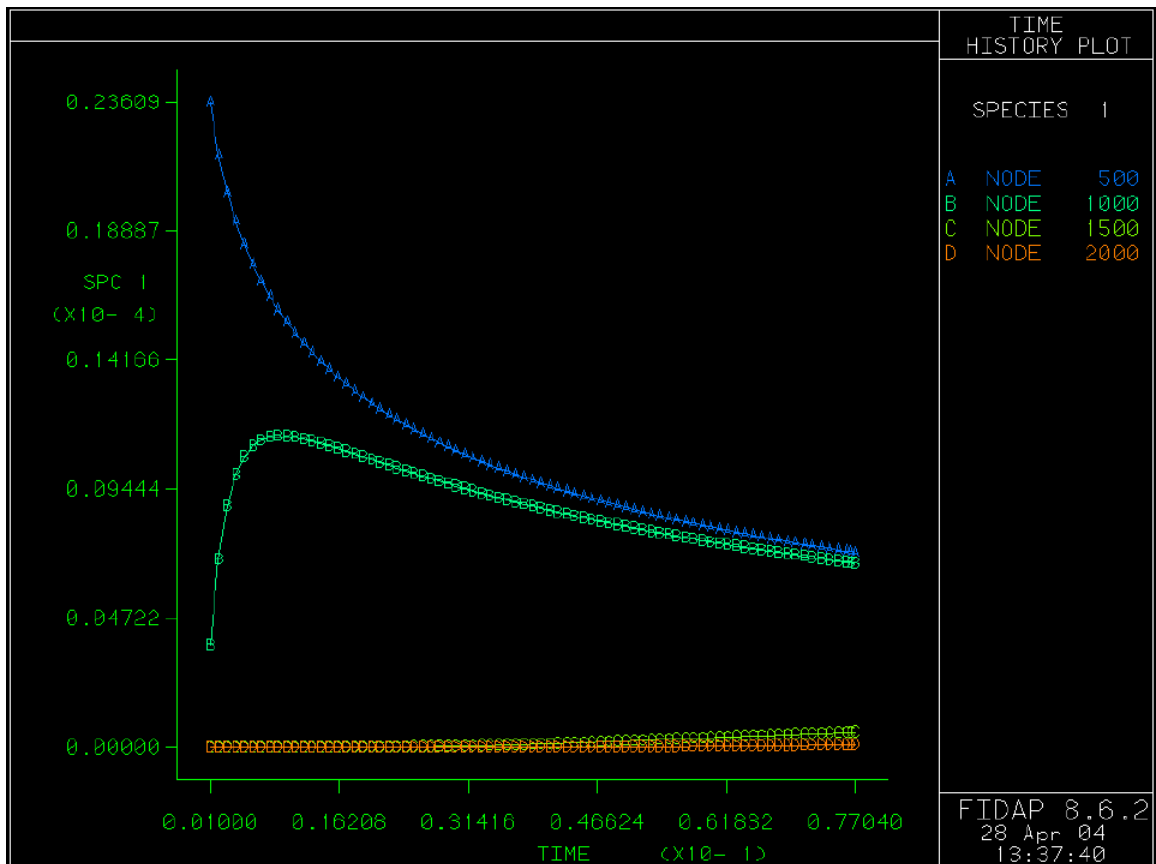


Figure 8B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Enamel diffusivity = $\frac{1}{4}$ * original value = $1.95 \times 10^{-11} \text{ m}^2/\text{s}$.

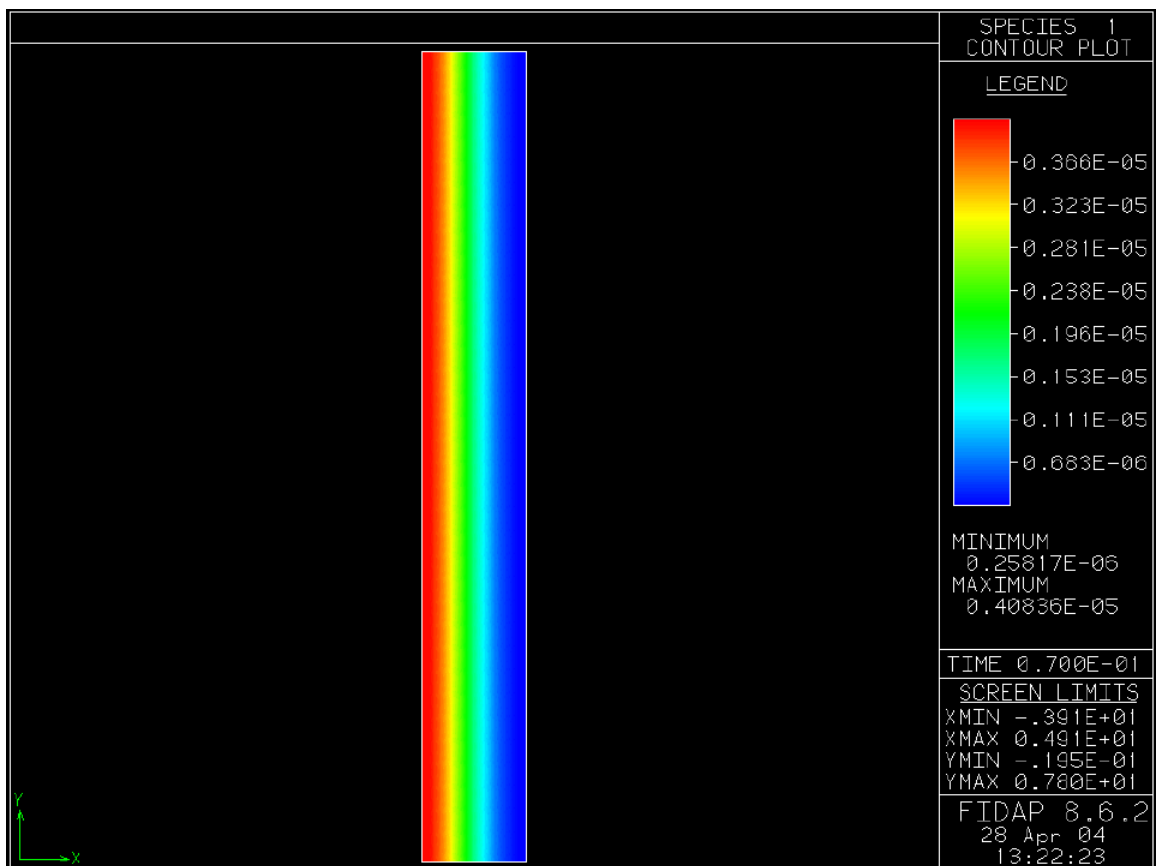


Figure 9A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Diffusivity of enamel = original value = $7.8 \times 10^{-11} \text{ m}^2/\text{s}$.

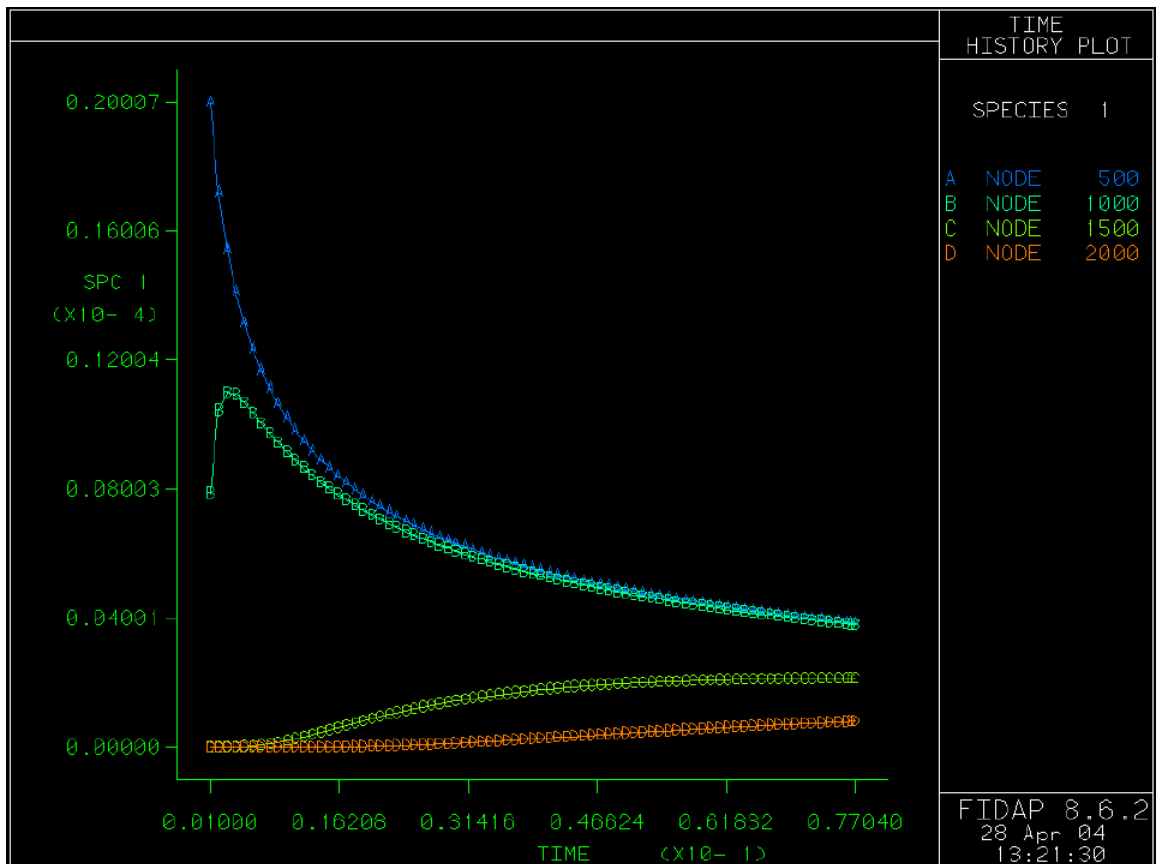


Figure 9B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Enamel diffusivity = original value = $7.8 \times 10^{-11} \text{ m}^2/\text{s}$.

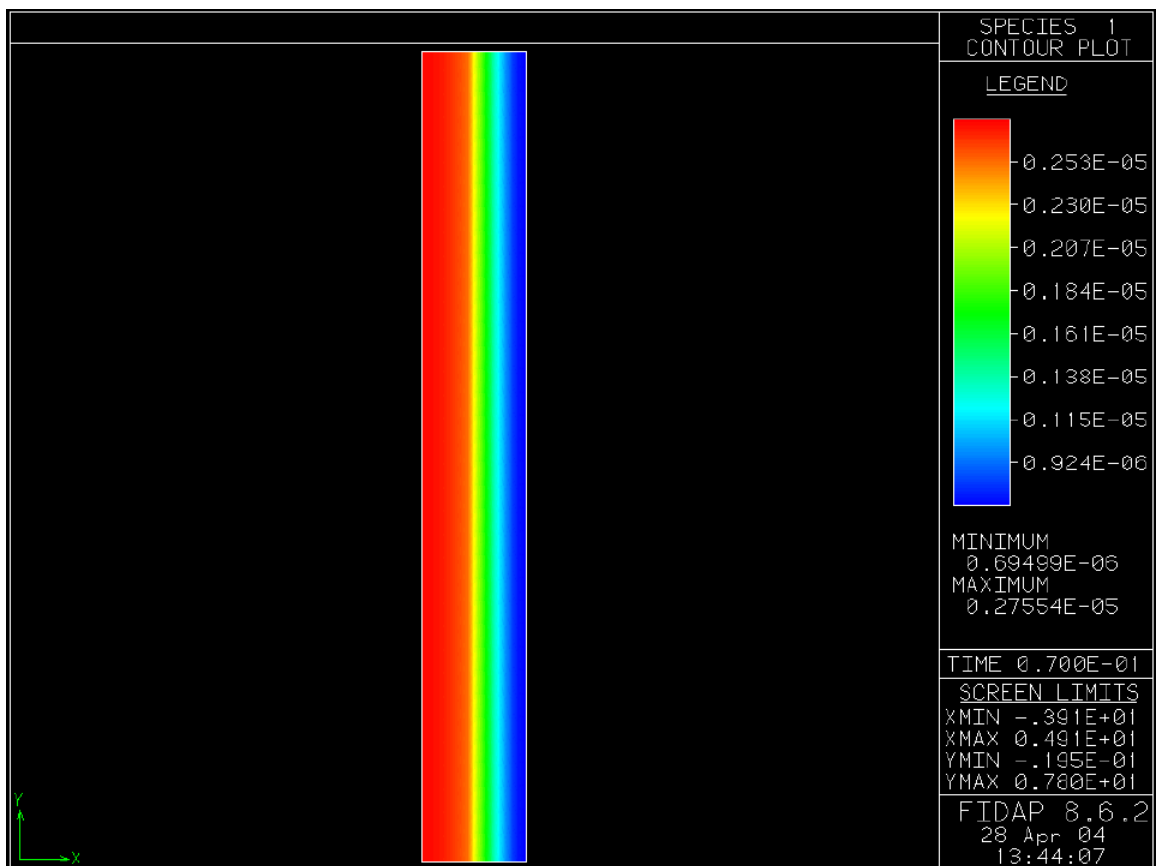


Figure 10A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Diffusivity of enamel = 5* original value = $3.9 \cdot 10^{-10} \text{ m}^2/\text{s}$.

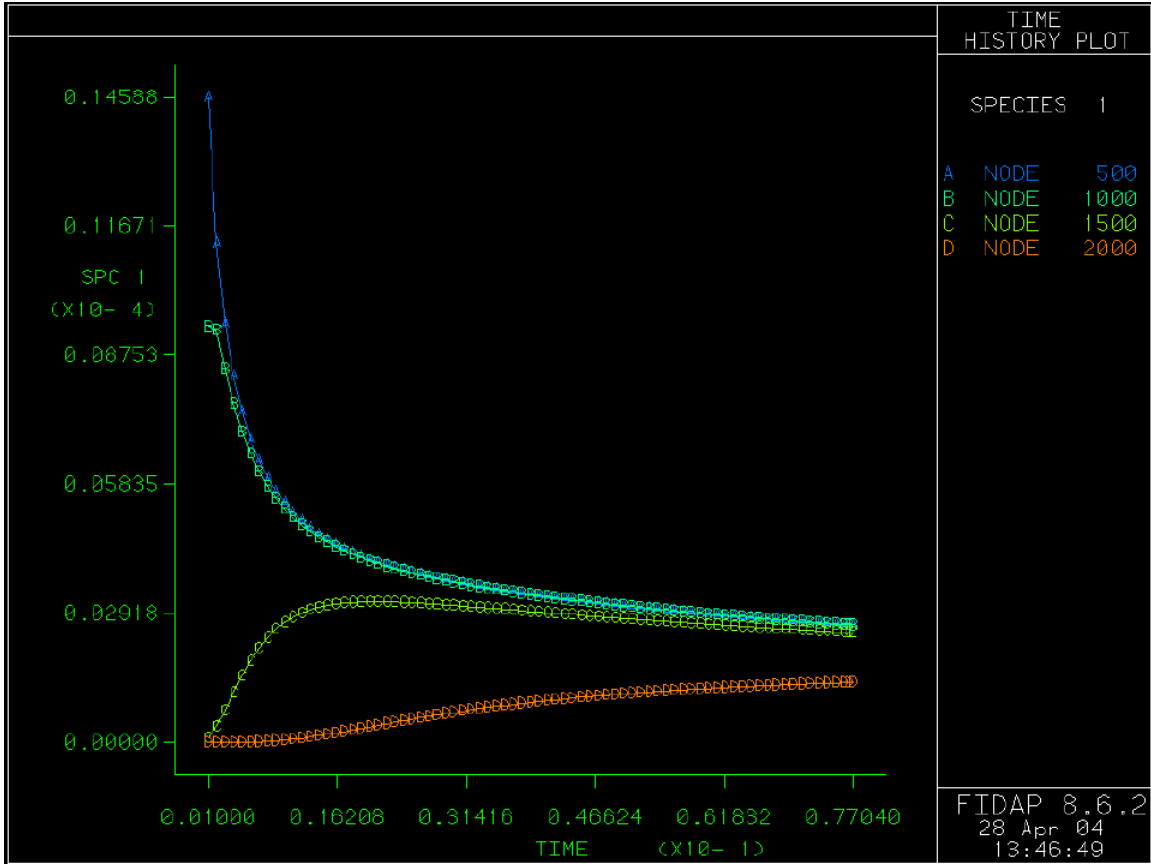


Figure 10B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Enamel diffusivity = $5 \times \text{original value} = 3.9 \times 10^{-10} \text{ m}^2/\text{s}$.

From these figures, we see similar trends to those seen by varying the dentin diffusivity. As the enamel diffusivity is increased, the concentration of hydrogen peroxide in gel decreases while the hydrogen peroxide in both the enamel and dentin increase (seen in Figure 10). This makes sense since the hydrogen peroxide will be able to diffuse much more easily at through the enamel when the diffusion coefficient in the enamel is higher. As a result, more hydrogen peroxide will reach the dentin and so the concentration in the dentin will be higher as well, although not as high as that in the enamel. On the other hand, as the enamel diffusion coefficient is decreased, the hydrogen peroxide will remain in the gel for a longer amount of time and the diffusion process will take a much longer time (see Figure 8). This is the more realistic case since the enamel is harder than the dentin.

Figures 11 through 14 show the diffusion of hydrogen peroxide through the gel and tooth layers as the reaction rate for the hydrogen peroxide reaction rate in the enamel and dentin was varied by orders of magnitude while all the other properties were kept constant. The reaction rate value was varied from 5.5×10^{-2} to $5.5 \times 10^5 \text{ M/s}$. The original reaction rate value was $5.5 \times 10^1 \text{ M/s}$. The contours and plots for the reaction rates of 5.5×10^{-2} to $5.5 \times 10^1 \text{ M/s}$ were approximately equal so we chose to use the contour and plot

for the reaction rate of $5.5 \cdot 10^1$ M/s, our original reaction rate, to represent this group of solutions in the report. Additionally, we chose to include the reaction rates $5.5 \cdot 10^2$ M/s and $5.5 \cdot 10^3$ M/s since the most dramatic changes occurred between these two graphs. Finally, we included the graphs for the reaction rate of $5.5 \cdot 10^5$ M/s since it represents the upper limit extreme.

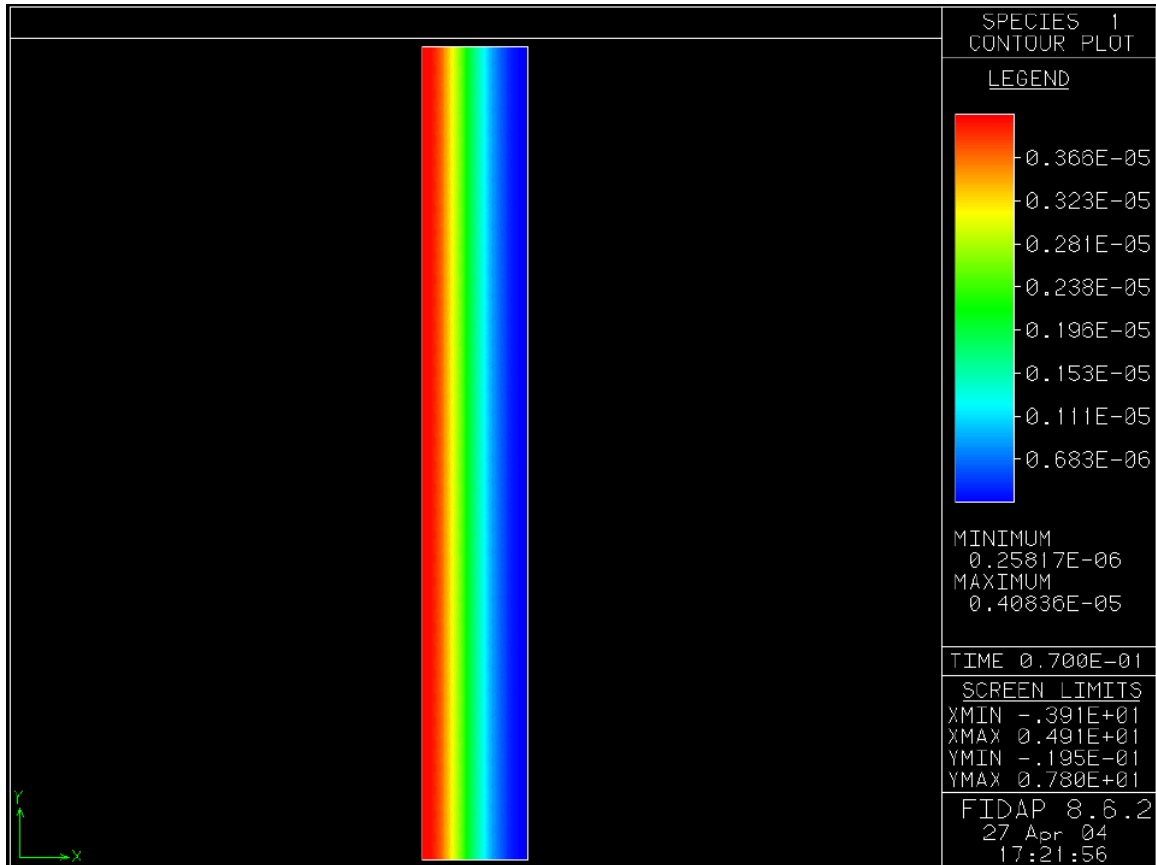


Figure 11A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Reaction rate = $5.5 \cdot 10^1$ M/s.

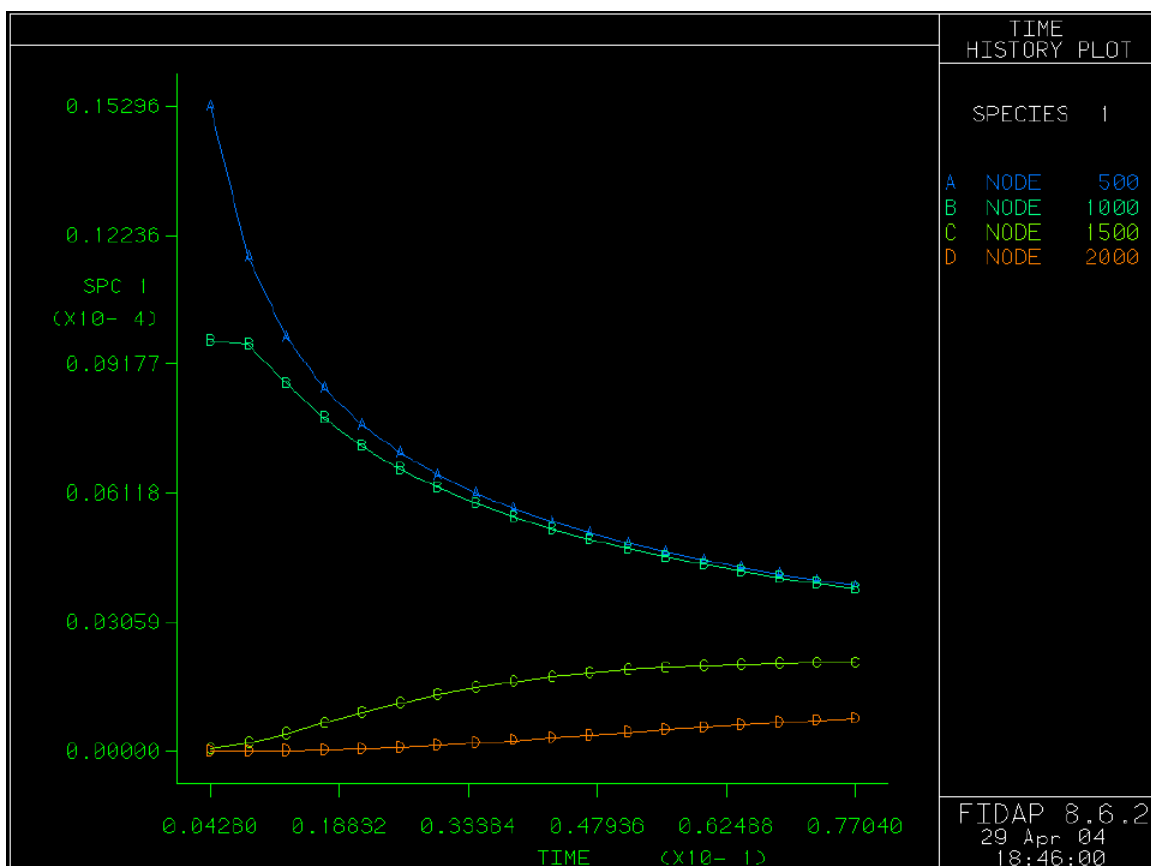


Figure 11B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Reaction rate = 5.5×10^1 M/s.

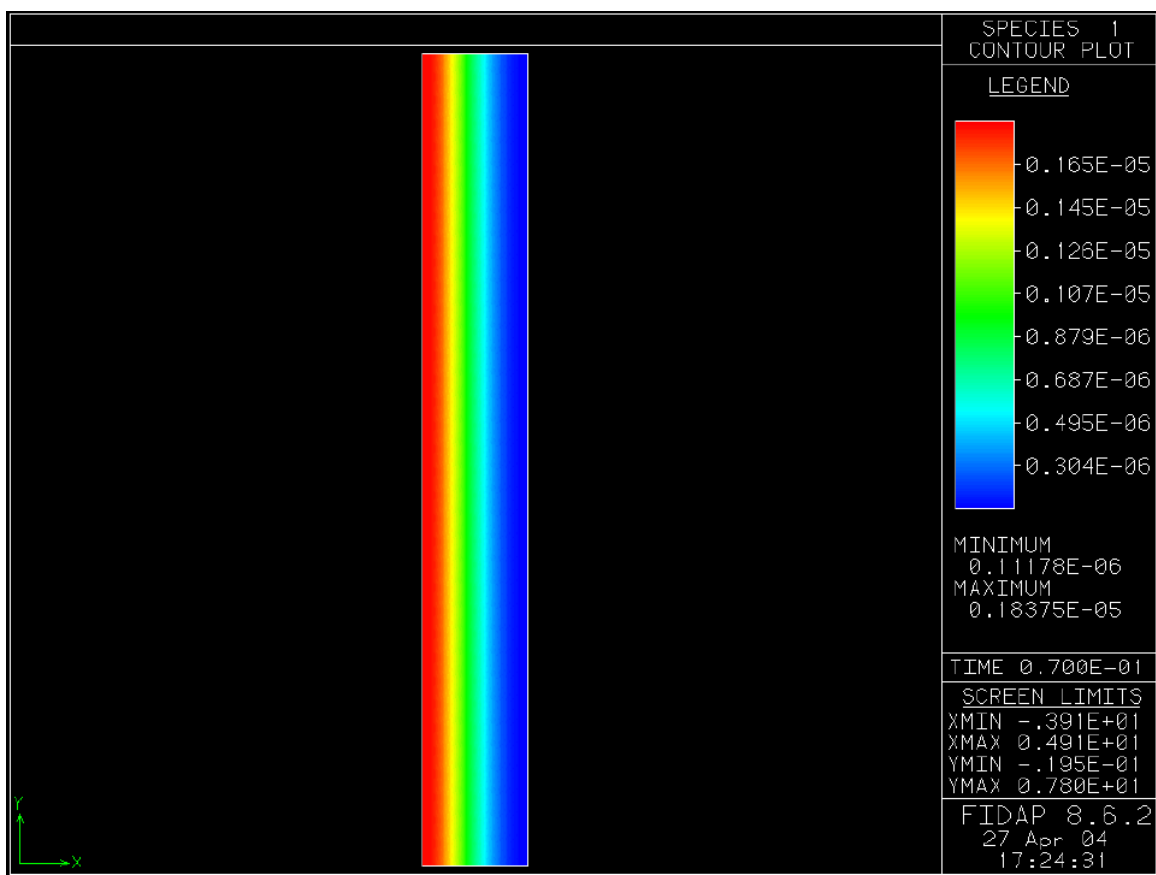


Figure 12A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Reaction rate = 5.5×10^2 M/s.

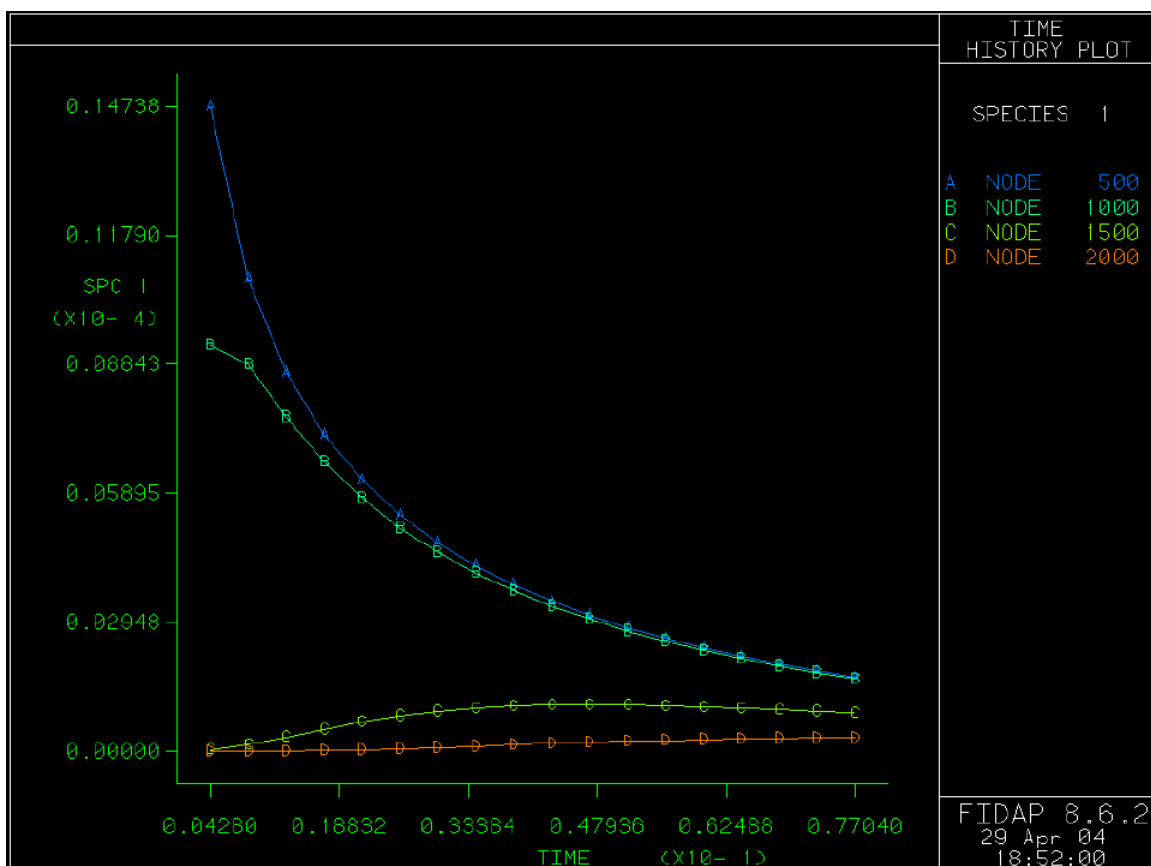


Figure 12B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Reaction rate = 5.5×10^2 M/s.

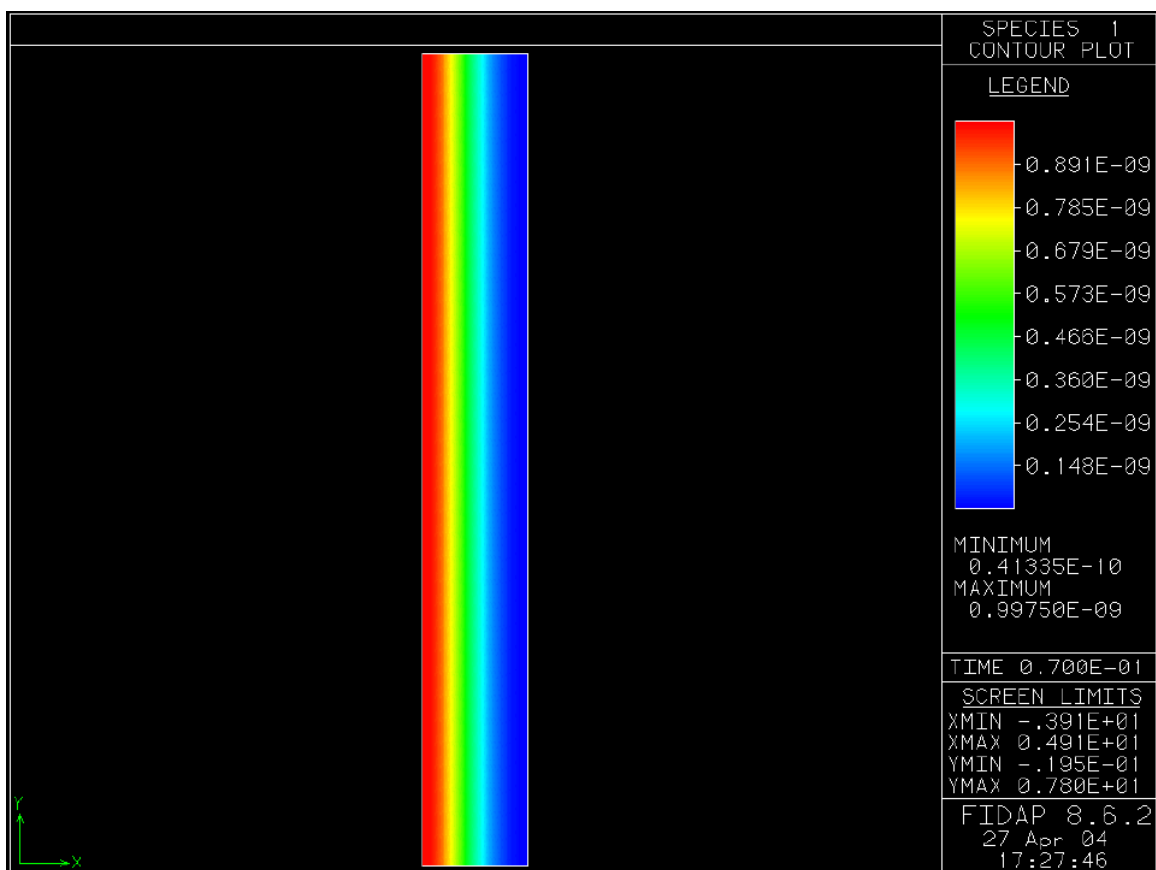


Figure 13A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Reaction rate = 5.5×10^3 M/s.

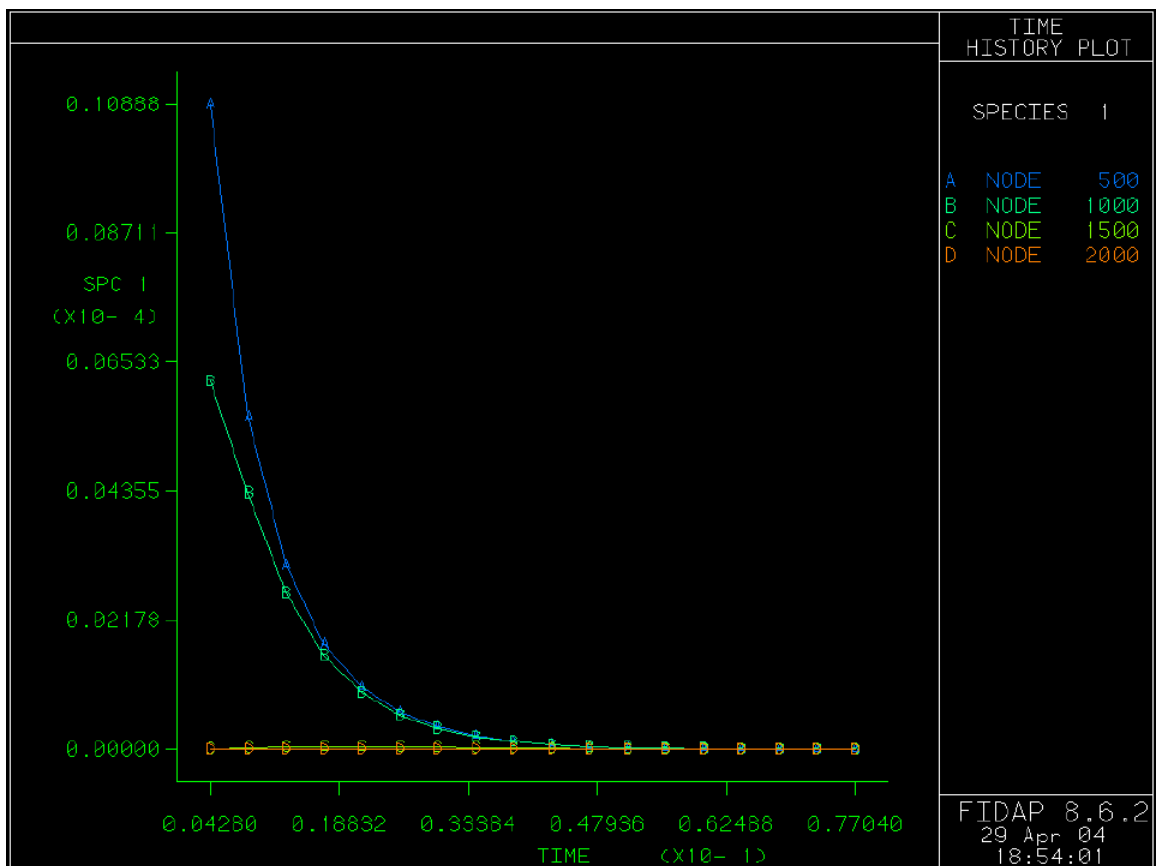


Figure 13B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Reaction rate = 5.5×10^3 M/s.

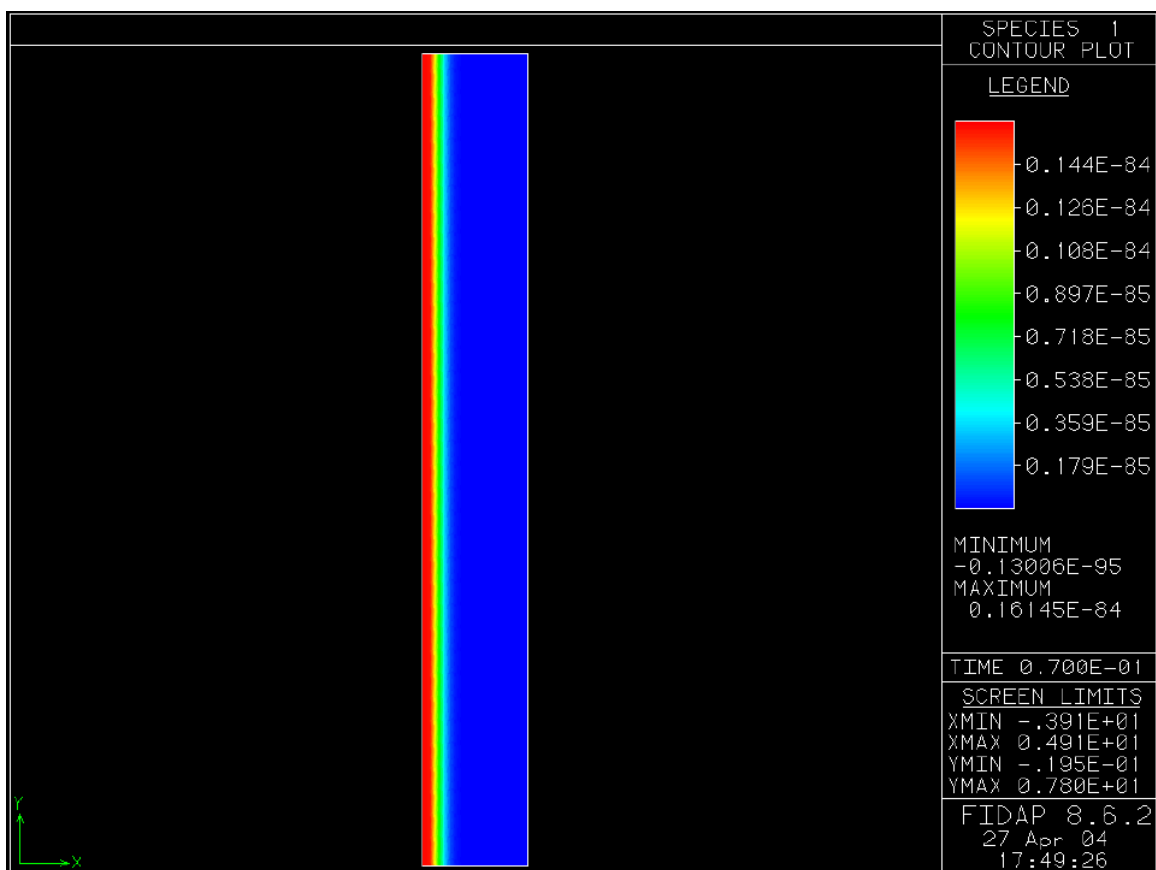


Figure 14A: Contour plot displaying diffusion of hydrogen peroxide through gel, enamel, and dentin (from left to right). Reaction rate = 5.5×10^5 M/s.

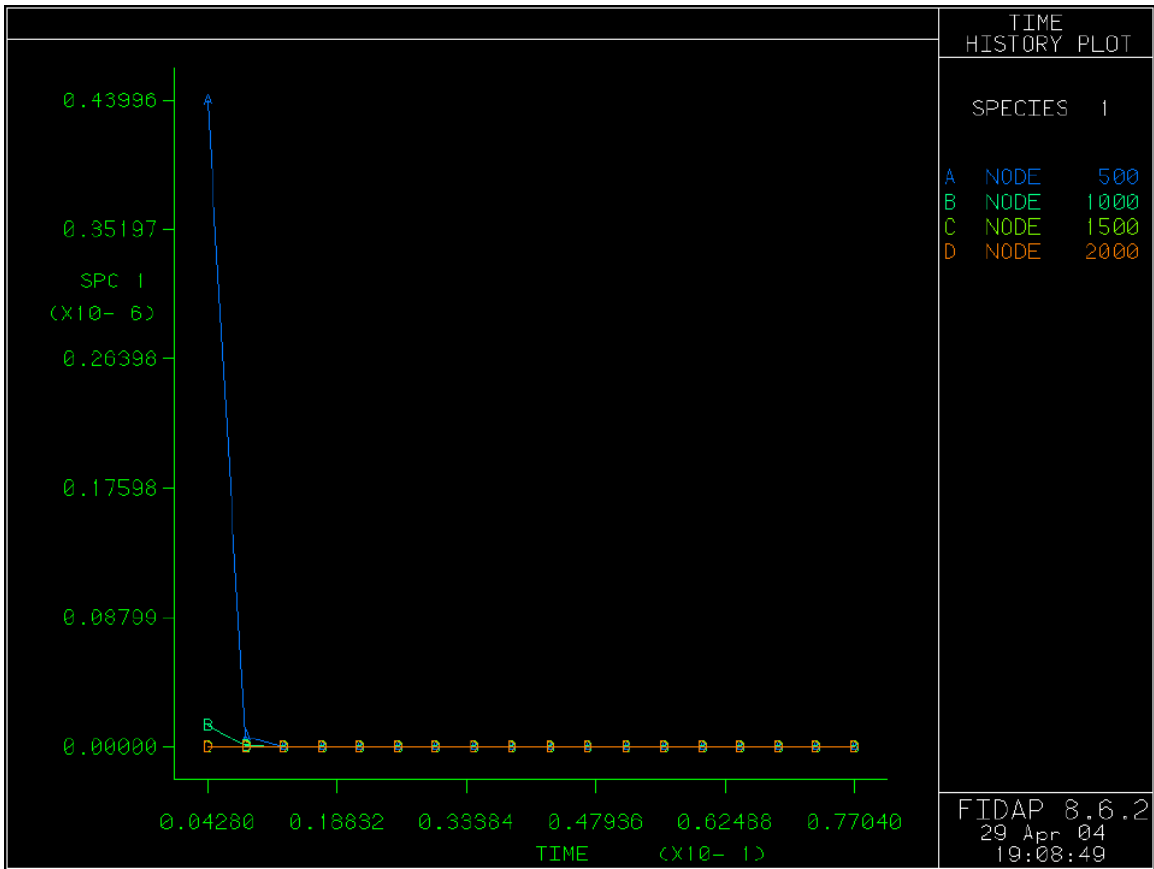


Figure 14B: Plot displaying the concentration of hydrogen peroxide [g/L] versus non-dimensional time. Node A is located in the gel. Node B is located on the left edge of the enamel. Node C is located in the enamel. Node D is located in the dentin. Reaction rate = 5.5×10^5 M/s.

From these figures, it is apparent that the order of magnitude of the reaction rate has a huge impact on the solution found. Looking in order from Figure 11 to Figure 14, as the reaction rate is increased, the concentration of hydrogen peroxide in the gel, enamel, and dentin decreases because so much of the hydrogen peroxide is being used up very quickly with high reaction rates.

From the sensitivity analysis conducted in this study, it is clear that the solution is dependent on using the correct values for both the diffusion coefficient and the reaction rate.

Conclusions and Design Recommendations:

Our model shows that hydrogen peroxide does in fact diffuse through the enamel and dentin in 30 minutes. Both the diffusion coefficient and reaction rate highly affect the solution, and therefore, accurate values of both must be used in order to obtain an accurate solution. A possible safety concern could emerge if the strips are left on for a much longer than 30 minutes. If the hydrogen peroxide further diffuses into the pulp of the teeth, the innermost layer of the tooth, the teeth could ache from sensitivity. The

environment might be affected by the use of white strips because they are disposable plastic strips. Since the strip is not reused, it is just thrown in the garbage, contributing to the large amount of waste that takes up much space in the world. A better idea may be for Crest to sell the gel, which could be applied to a re-usable plastic strip.

White strips are a cost-effective alternative to expensive whitening methods that require a trip to the dentist. The effectiveness of the white strips was modeled using the finite element analysis program, FIDAP, by the diffusion of hydrogen peroxide through the tooth layers. Therefore, we recommend the use of white strips to all consumers looking to “put their best teeth forward.”

Appendix A:

Geometry:

Please refer to the schematic shown in Figure 3.

The following selections were chosen to define the problem definition: 2-D geometry, transient simulation, no-momentum equation, and species dependence. 2-D geometry was used since the 3 layers (gel, enamel, and dentin) were modeled as a flat, finite plate. Alternately, we could have simplified our model by using an axi-symmetric geometry due to the axis of symmetry (x-axis). A transient solution to the diffusion equation was used because the concentration of hydrogen peroxide in the gel and in the tooth layers change with time. Finally, the momentum equation was not utilized since there was no relevant fluid movement.

Governing Equation:

Diffusion equation without velocity

$$\frac{\partial c_A}{\partial t} = D \frac{\partial^2 c_A}{\partial x^2} + r_A$$

Where:

- c_A = concentration of hydrogen peroxide
- D = diffusion coefficient of hydrogen peroxide through tooth
- r_A = the mass degradation rate of the hydrogen peroxide as it is used up in chemical reaction

Boundary Conditions:

1. At $x = 0$ and $x = 0.00135$ m, $dc/dx = 0$
2. At $y = 0$ and $y = 0.0105$ m, $dc/dx = 0$

Initial Conditions:

1. At $t = 0$, $c(\text{for all } x \text{ in "Enamel"}) = 0$
2. At $t = 0$, $c(\text{for all } x \text{ in "Dentin"}) = 0$
3. At $t = 0$, $c(\text{for all } x \text{ in "Gel"}) = 2.8 \times 10^{-5} \text{ g/L}$

Properties:

	Diffusion coefficient (D) [m^2/s]	Source # (see References)
Gel	$1.3 \cdot 10^{-9}$	6
Enamel	$7.8 \cdot 10^{-11}$	1
Dentin	$7.8 \cdot 10^{-11}$	1

	Reaction rate (r_A) [M/s]	Source # (see References)
Gel	0	2
Enamel	Very low	5
Dentin	Very low	5
Tooth Stains	$5.5 \cdot 10^9$	3

The concentration of H_2O_2 on the white strips → Source #4

Thickness of strip, length, width and amount of whitening gel → Source #8

Appendix B:

(a) PROBLEM statement keywords

Geometry type	2-D	3 layers were modeled as flat, finite plate.
Flow regime	Incompressible	The contents are incompressible.
Simulation type	Transient	The concentration depends on time.
Flow type	Laminar	The flow is laminar.
Convective term	Linear	There is no convection.
Fluid type	Newtonian	The system behaves in a Newtonian manner.
Momentum equation	No momentum	There is no momentum in the tooth or gel.
Temperature dependence	Isothermal	Temperature is constant.
Surface type	Fixed	The surface is fixed.
Structural solver	No structural	There is no structural solver.
Elasticity remeshing	No remeshing	There is no remeshing.
Number of phases	Single phase	There is only matter in a single phase.
Species dependence	Species = 1	There is one species (hydrogen peroxide).

(b) SOLUTION statement keywords

Solution method	Steady state = 10	This sets the program to solve a steady state problem with a maximum of 10 iterations for any one time step.
Relaxation Factor	ACCF = 0	

(c) *TIMEINTEGRATION* statement keywords

Time integration	Backward	This specifies the time integration method for a transient analysis.
No. time steps	Nsteps = 100	The maximum number of discrete time integration steps to be calculated is 100.
Starting time	Tstart = 0	The starting time is 0.
Ending time	Tend = 0.07704	The ending time is 0.07704 (non-dimensional = $Do \cdot t / L^2$)
Time increment	Dt = .00428	The time increment is 0.00428 (non-dimensional = $Do \cdot \Delta t / L^2$)
Time stepping algorithm	Fixed	The time increment is fixed.

Mesh:

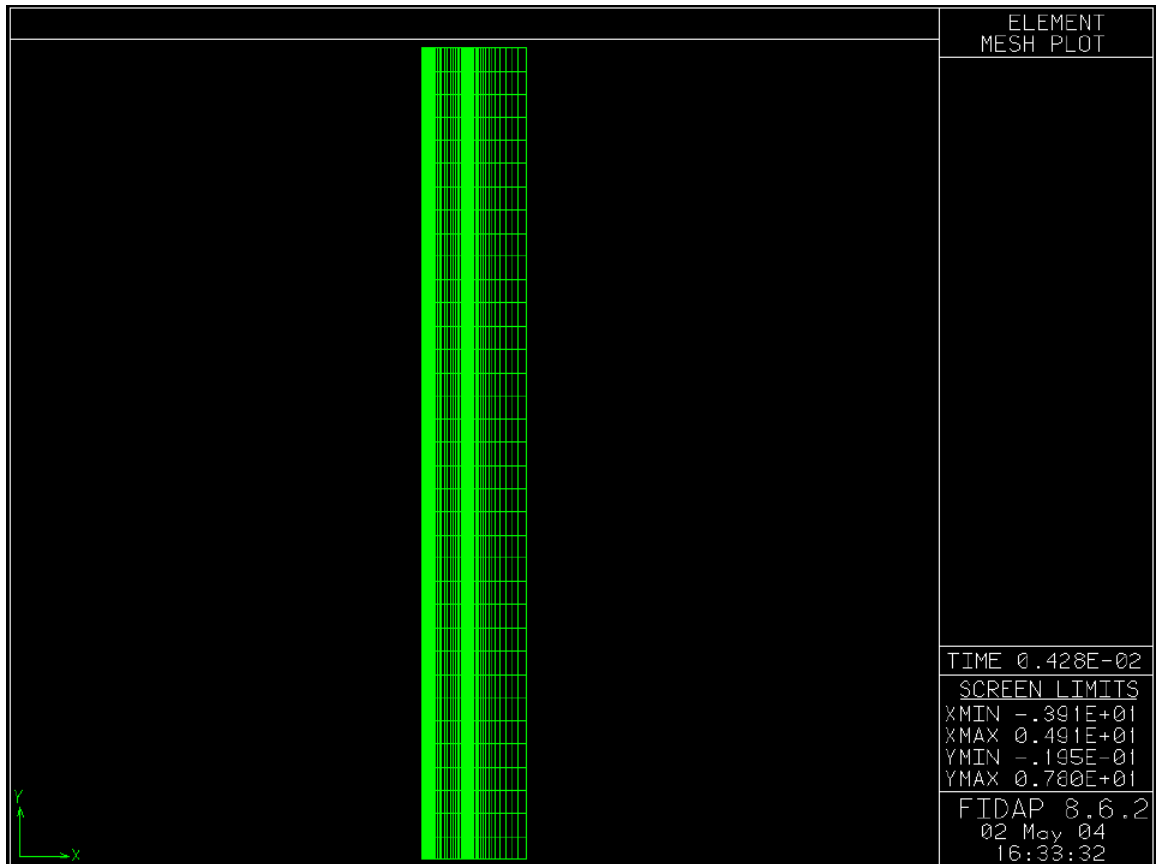


Figure 15: Final mesh

Convergence Analysis:

We conducted a convergence analysis on our mesh in order to see which mesh would give us the most accurate solution and allow the least running time. We tried using many meshes but will only present the findings of three in this report (Table 1).

Table 1: The number of nodes for each layer as well as total number of nodes used in the three meshes we used to find mesh convergence.

Mesh #	# of Gel Nodes	# of Enamel Nodes	# of Dentin Nodes	Total # of Nodes
1	300	400	400	1100
2*	700	875	875	2450
3	960	1120	1120	3200

Figures 16-18 show the three contour plots for the three meshes we tried.

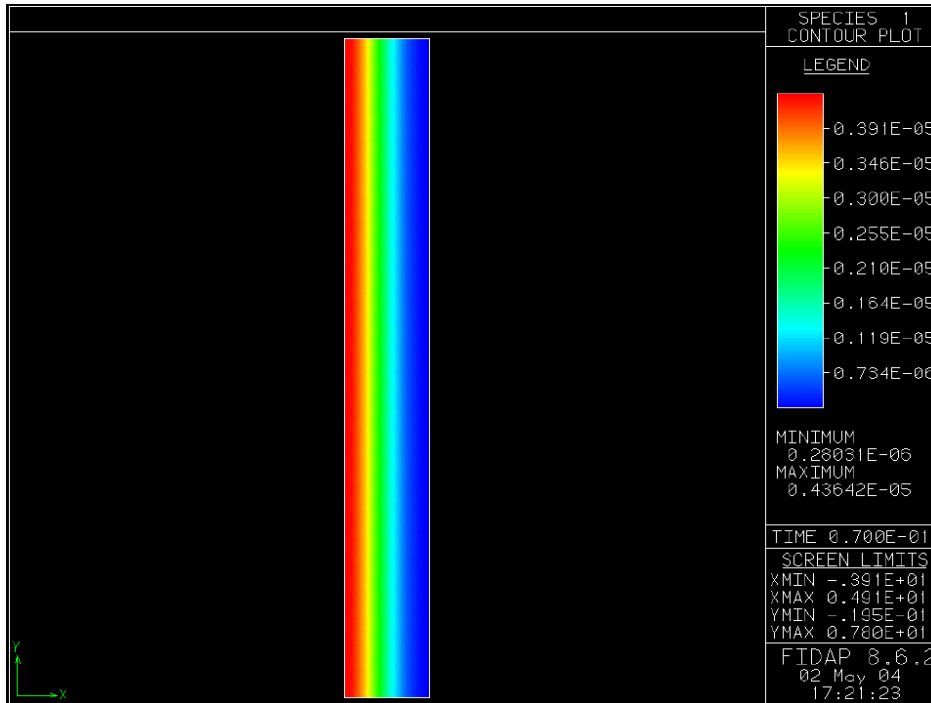


Figure 16: Contour plot of solution found when using a mesh with total number of nodes equal to 1100 nodes.

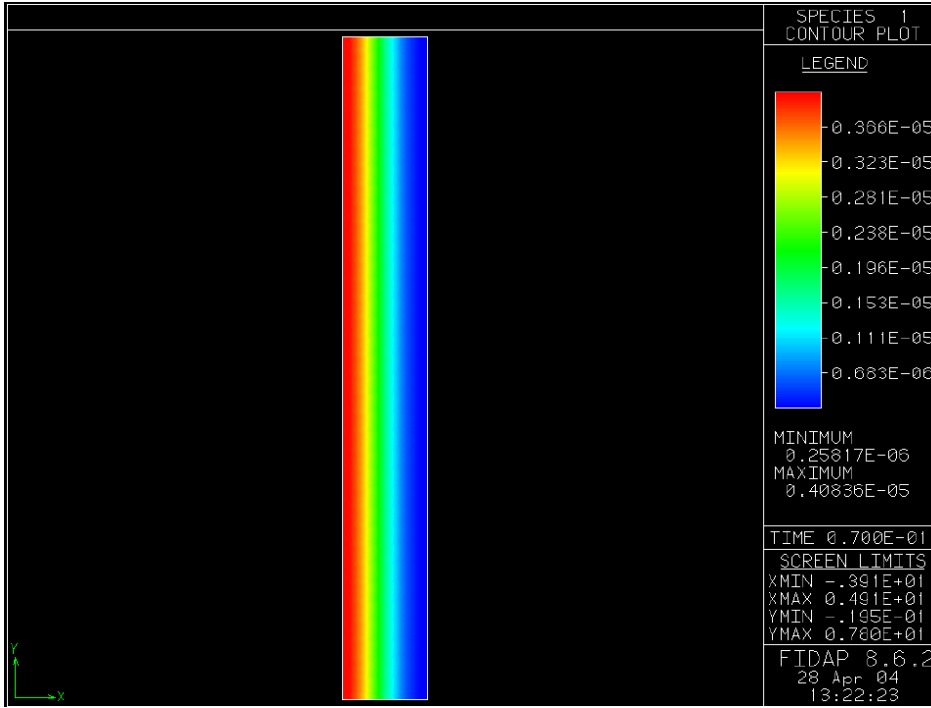


Figure 17: Contour plot of solution found when using a mesh with total number of nodes equal to 2450 nodes. This is the mesh we used in our final solution.

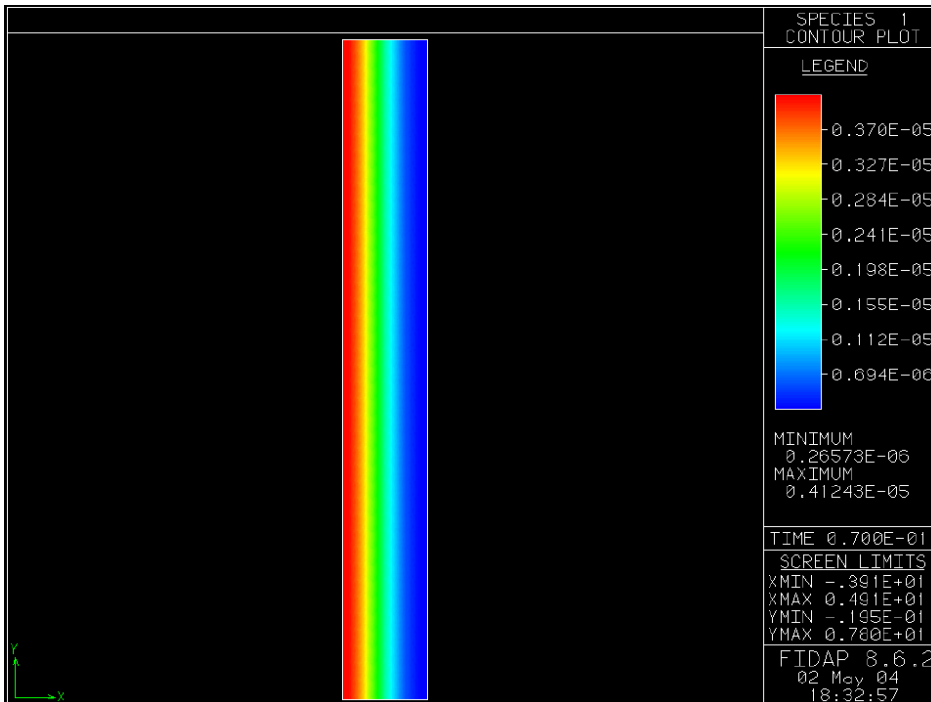


Figure 18: Contour plot of solution found when using a mesh with total number of nodes equal to 2450 nodes. This is the mesh we used in our final solution.

From these figures, it is apparent that the contour plots in Figures 17 and 18 are almost identical and therefore the mesh with 2450 nodes is the best choice since it will give just as accurate of a solution as Mesh #3, but will take less time to run in FIDAP.

FIDAP Input File

```
/ FICONV(NEUTRAL,NORESULTS,INPUT)
/ INPUT(FILE= "meg.FDNEUT")
/ END
/ *** of FICONV Conversion Commands
/
TITLE

/
/ *** FIPREP Commands ***
/
FIPREP
PROB (2-D, INCO, TRAN, LAMI, LINE, NEWT, NOMO, ISOT, FIXE, NOST, NORE,
SING,
    SPEC = 1.0)
EXEC (NEWJ)
SOLU (S.S. = 10, ACCF = 0.000000000000E+00)
TIME (BACK, NSTE = 1, TSTA = 0.000000000000E+00, TEND = 0.770400000000E-
01,
    DT = 0.428000000000E-02, FIXE)
ENTI (NAME = "Gel", SOLI, SPEC = 1.0, MDIF = "Gel")
ENTI (NAME = "Enamel", SOLI, SPEC = 1.0, MDIF = "Enamel", SPEC = 1.0, MREA
= 1)
ENTI (NAME = "Dentin", SOLI, SPEC = 1.0, MDIF = "Dentin", SPEC = 1.0, MREA =
1)
ENTI (NAME = "LeftGel", PLOT)
ENTI (NAME = "GelEnamel", PLOT)
ENTI (NAME = "EnamelDentin", PLOT)
ENTI (NAME = "BotGel", PLOT)
ENTI (NAME = "BotEnamel", PLOT)
ENTI (NAME = "BotDentin", PLOT)
ENTI (NAME = "RightDentin", PLOT)
ENTI (NAME = "TopDentin", PLOT)
ENTI (NAME = "TopEnamel", PLOT)
ENTI (NAME = "TopGel", PLOT)
DIFF (SET = "Enamel", CONS = 1.0)
DIFF (SET = "Dentin", CONS = 1.0)
DIFF (SET = "Gel", CONS = 16.667)
REAC (SET = 1, CONS, TERM = 1, KINE)
-0.5500000000E+05, 0.0000000000E+00, 0.0000000000E+00, 0.1000000000E+01,
0.0000000000E+00, 0.0000000000E+00, 0.0000000000E+00, 0.0000000000E+00,
0.0000000000E+00, 0.0000000000E+00, 0.0000000000E+00, 0.0000000000E+00,
```

```
0.0000000000E+00, 0.0000000000E+00, 0.0000000000E+00, 0.0000000000E+00,  
0.0000000000E+00, 0.0000000000E+00, 0.2730000000E+03  
BCFL (SPEC = 1.0, ENTI = "RightDentin", CONS = 0.000000000000E+00)  
BCFL (SPEC = 1.0, ENTI = "TopDentin", CONS = 0.000000000000E+00)  
BCFL (SPEC = 1.0, ENTI = "TopGel", CONS = 0.000000000000E+00)  
BCFL (SPEC = 1.0, ENTI = "TopEnamel", CONS = 0.000000000000E+00)  
BCFL (SPEC = 1.0, ENTI = "BotGel", CONS = 0.000000000000E+00)  
BCFL (SPEC = 1.0, ENTI = "BotEnamel", CONS = 0.000000000000E+00)  
BCFL (SPEC = 1.0, ENTI = "BotDentin", CONS = 0.000000000000E+00)  
BCFL (SPEC = 1.0, ENTI = "LeftGel", CONS = 0.000000000000E+00)  
ICNO (SPEC = 1.0, ZERO, ENTI = "Enamel")  
ICNO (SPEC = 1.0, ZERO, ENTI = "Dentin")  
ICNO (SPEC = 1.0, CONS = 0.280000000000E-04, ENTI = "Gel")  
END  
/ *** of FIPREP Commands  
CREATE(FIPREP,DELE)  
CREATE(FISOLV)  
PARAMETER(LIST)
```

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