Comparison of oxygen flux in hydrogel and silicone hydrogel contact lenses

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Executive Summary:

The prevalence of contact lens use has been continuously growing for their convenience and for cosmetic reasons. Although contact lenses do offer many advantages over glasses, the major concern for many contact lens users is dryness that results from a lack of oxygen that goes through the contact lens to meet the demand of eye tissue. A new type of contact lens, made out of silicone hydrogel, has been introduced in the market which has garnered much attention from many contact users. The silicone hydrogel is different from the traditional hydrogel contact lens since oxygen is permeable through silicone, which was not possible through hydrogels. The hydrogel contact lenses must have high water content for oxygen delivery, silicone hydrogel contacts depends on their high oxygen diffusivity while having low water content. Night and day contact lenses are made out of silicone hydrogel whereas traditional ones for day use are often made out of hydrogel. A model was developed to validate the advantage of wearing silicone hydrogel contact lenses in both day and night conditions. By analyzing the center area of the eye around the pupil as a thin slab, the performance of these two types of contact lenses were compared by computing average oxygen concentrations in the stroma, which is the largest layer of cornea. Using COMSOL Multiphysics, the simplified geometry that included the layers of contact lens, tear, endothelium, and stroma was used as our model to find the oxygen concentration after eight hours of use either with eyes open or closed. The thickness of 80µm was used for both hydrogel and silicone hydrogel, the average oxygen concentration was found to be 9.100219×10^{-8} mol/cm^3 and 4.198608×10^{-8} mol/cm^3 respectively for day setting with eyes open for eight hours and 3.536442×10^{-8} mol/cm^3 and 2.119774×10^{-8} mol/cm^3 respectively for night setting with eyes closed. Variations of other parameters in modeling also showed the same trend that silicone hydrogel contact lenses ended up with less oxygen in the cornea than hydrogel. Thus, the modeling showed how the silicone hydrogel did not offer any increase in oxygen delivery in both day and night settings.

Key words: silicone hydrogel contact lenses, oxygen permeability

Introduction

Contact lenses have become a popular alternative choice for many people who, otherwise, have to wear glasses for the correction of their vision. There are many different types of contact lenses, but the two main categories are hard and soft lenses. Although there are advantages and disadvantages for both types of contact lenses, the demand is higher for soft contacts due to their ease of use. Within the category of soft contact lens, there are different types and manufacturers that vary in water content, shape, materials, and the duration of use. A great majority of contact lens users wear disposable contact lenses that need to be taken out before sleeping. In the current market, however, there are night and day soft contact lenses available that can be worn continuously for a month long period without daily removal.

Focus Night and Day contact lenses are made out of silicone hydrogel, which is considered as a revolutionary change to previous hydrogel contact lenses, as oxygen is permitted through the silicone unlike hydrogel. 1-Day Acuvue contact lenses are made out of hydrogel polymer, which does not permit direct oxygen diffusion. In hydrogel contact lenses oxygen diffuses directly through the water within the material. Alternatively, silicone hydrogels have a lower water content yet a higher diffusivity because silicone is more permeable than water to oxygen [Efron *et al*].

Contact lens users may take a nap or go to bed with their contact lenses on their eyes. Wearing traditional hydrogel contact lenses during sleep, however, makes the eyes feel extremely dry afterwards. Contact lenses become stiff and can even pop out of the eyes in extreme cases. The manufacturers of silicone hydrogel contact lenses promote the ability to wear their contact lenses for many consecutive days without having to take them out every night. In order to compensate for such continuous use, the silicone hydrogel contact lenses must have unique properties that could result in a range of comfortable oxygen concentrations in the cornea.

When the silicone hydrogel contact lenses were first introduced in the market, the main focus of the advertisement was their high diffusivity of oxygen. Such attention-grabbing marketing of silicone hydrogel contact lenses made many consumers think choosing silicone hydrogel contact lenses over traditional hydrogel ones could help them avoid dryness and discomfort that contact lenses often cause. Through our modeling experiments, we want to verify whether these claims are true.

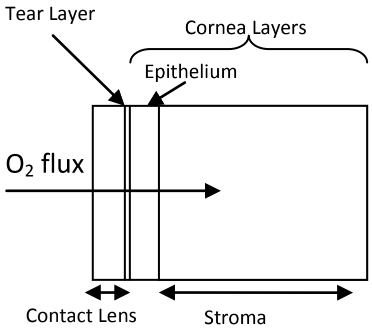
Design Objectives:

We are interested in comparing whether silicone hydrogel contact lenses are more beneficial than hydrogel contact lenses for daily use. The use of a specific contact lens is beneficial if the concentration of oxygen in the stroma is continuously above the threshold of 12.1% of atmospheric oxygen conditions throughout the eight hour comparison. Additionally, we hope to determine if the silicone hydrogel contact lenses are beneficial for overnight use, based on an eight hour comparison to hydrogel contact lenses.

Problem Schematic:

In order to meet our objectives, the center of the eye is modeled as a thin slab. The four layers included in the model are the contact lens, the tear layer, the epithelium, and the stroma. The schematic, shown on the following page, depicts the direction of oxygen flow and relative position of each layer. The governing equation and the boundary and initial conditions are also listed on the same page.

Schematic:



-- For Boundary conditions, please see below.

Thickness Dimensions of Schematic:
Contact lens = .008 cm
Tear layer = .0003 cm
Epithelium = .005 cm
Stroma = .048 cm

*Note: This models 1D oxygen flow only. Therefore the width is arbitrary, but set to .005 cm in this case.

Governing equation:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - R_A$$

Boundary Conditions and Initial Conditions:

Lens:	Focus Night & Day
Water Content:	24%

Eye Open Conditions		Eye Closed Conditions	
Initial:	[mol/cm^3]	Initial:	[mol/cm^3]
Contact Lens	6.552E-08	Contact Lens	6.552E-08
Cornea	6.552E-08	Cornea	6.552E-08
Boundary:		Boundary:	
c(x=0) - back of cornea	4.105E-08	c(x=0) - back of cornea	4.105E-08
c(x=.0613) - end of contact	6.552E-08	c(x=.0613) - end of contact	2.228E-08

Lens:	1Day Acuvue
Water Content:	58%

Eye Open Conditions		Eye Closed Conditions	
Initial:	[mol/cm^3]	Initial:	[mol/cm^3]
Contact Lens	1.583E-07	Contact Lens	1.583E-07
Cornea	1.583E-07	Cornea	1.583E-07
Boundary:		Boundary:	
c(x=0) - back of cornea	4.105E-08	c(x=0) - back of cornea	4.105E-08
c(x=.0613) - end of contact	1.583E-07	c(x=.0613) - end of contact	5.384E-08

For all other boundaries, Flux = 0.

Results and Discussion:

After implementing these conditions in COMSOL, the average concentrations in the stroma were determined through subdomain integration of the concentration in the stroma. During daytime use, with an open eye, the silicone hydrogel had an average oxygen concentration in the stroma of $4.20\text{x}10^{-8}$ mol/cm^3, while the hydrogel had an average oxygen concentration in the stroma of $9.10\text{x}10^{-8}$ mol/cm^3. The hydrogel allowed the stroma to have on average over two times the level of oxygen found when using a silicone hydrogel. Our results show that this may not be severely detrimental to eye health, while the silicone hydrogel provides a great deal of more discomfort than the hydrogel lens. The simulated average oxygen concentration of the stroma of a non-contact wearer was roughly $1.7\text{x}10^{-7}$ mol/cm^3, suggesting that both lenses severely restricted oxygen flux to certain regions of the eye. This is why wearing any lens can bring discomfort to new contact lens users. The oxygen concentration in the stroma for hydrogel contact lens users is 54% of the concentration when no contact lens is worn. Although the oxygen concentration in the stroma for silicone hydrogel contact lenses is expected to be higher than that of the hydrogels, the silicone hydrogel's oxygen concentration is less than 25% of the value recorded without a contact lens. This explains why silicone hydrogel users often complain of discomfort in daily wear.

As seen below, Figure 2 displays the concentration profile in the depth of the cornea. The left side represents the end of the stroma, while the right end represents the contact surface exposed to the air.

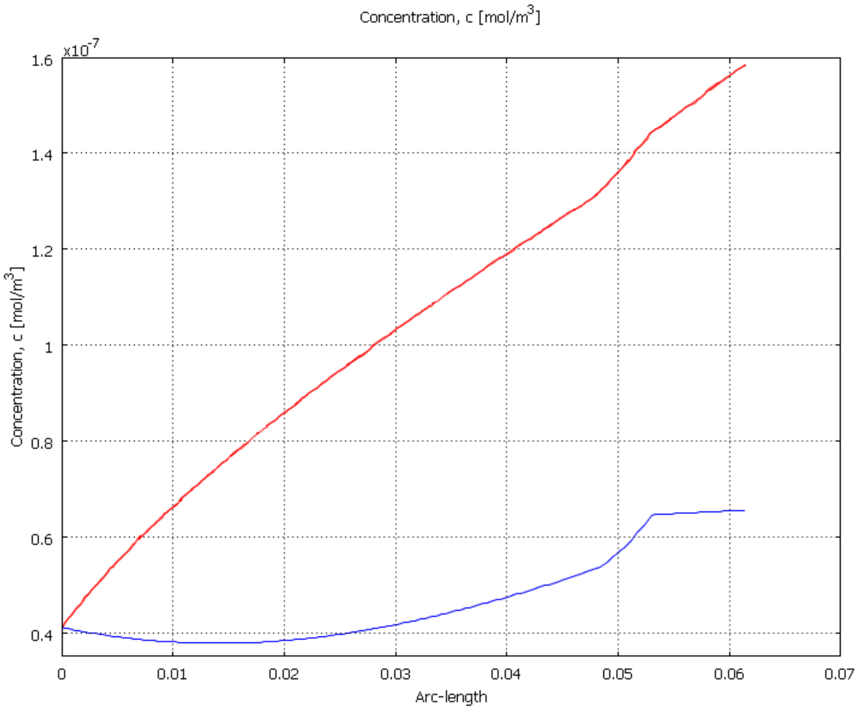


Fig. 2: Concentration contours over the length of the lens during day wear of regular hydrogel (red) and silicone hydrogel (blue) in mol/cm^3.

Based on Figure 2, the hydrogel contact lens decreases relatively consistently from the lens to the back of the cornea, in a linear fashion. The silicone hydrogel, however, is largely affected by the degradation rate in the stroma. Although the oxygen concentration decreases very little while still in the contact lens, the concentration drops quickly near the stroma-epithelium border. In both cases, the oxygen concentration does not decrease to a level much less than the concentration near the back of the stroma, due to blood flow. As a result, it is very unlikely that major tissue damage will occur due to lack of oxygen, as the values at the minimum are basically equivalent to this boundary. Due to a large difference in concentration between the hydrogel and silicone hydrogel at comparable locations throughout the stroma, it is clear that the hydrogel lens provides less discomfort resulting from lack of oxygen.

Yet, the problem is not solved at night, either. Overnight wear of contact lenses of any kind can greatly restrict oxygen flow to the eye, due to a decreased oxygen concentration at the boundary of the eye. By simulating conditions with the closed eye, with a value of 35% of the open eye contact-air boundary condition, it was found that the average concentration in the stroma for the hydrogel lens was $3.54x10^{-8}$ mol/cm^3. This was roughly a 60% drop from the eye open condition. As seen in Figure 3, the hydrogel, represented by the red line, never decreases to a concentration close to zero, but it is significantly lower than concentrations expressed during the day. Likewise, a concentration of 12.1% of atmospheric oxygen concentration, or $3.3x10^{-8}$ mol/cm^3, is required to limit corneal swelling. This will allow the cornea to recover to normal thickness soon after the eye opens, again [Holden]. Based on Figure 3, the minimum corneal concentration when wearing the hydrogel lens is roughly $3.3x10^{-8}$ or $3.4x10^{-8}$ mol/cm^3, suggesting that overnight use, while providing eye discomfort, does not severely damage the eye by causing irreversible swelling.

Unlike the regular hydrogel, the silicone hydrogel makes significant changes in its contour shape and concentration value. With an average concentration in the stroma of $2.12\ x10^{-8}$ mol/cm^3, the silicone hydrogel does not decrease nearly as much between day and night use as the hydrogel does, yet this value still represents a 50% decrease from the concentration determined during the day. As seen in Figure 3, the boundary condition at the lens of the silicone hydrogel is less than half the value of the hydrogel. Further, the concentration decreases until there is nearly no oxygen in certain parts of the stroma. When again comparing to the value representing limited corneal swelling, nearly the entire length of the eye is below this threshold. This can be extremely damaging over prolonged use, leading to irreversible eye swelling.

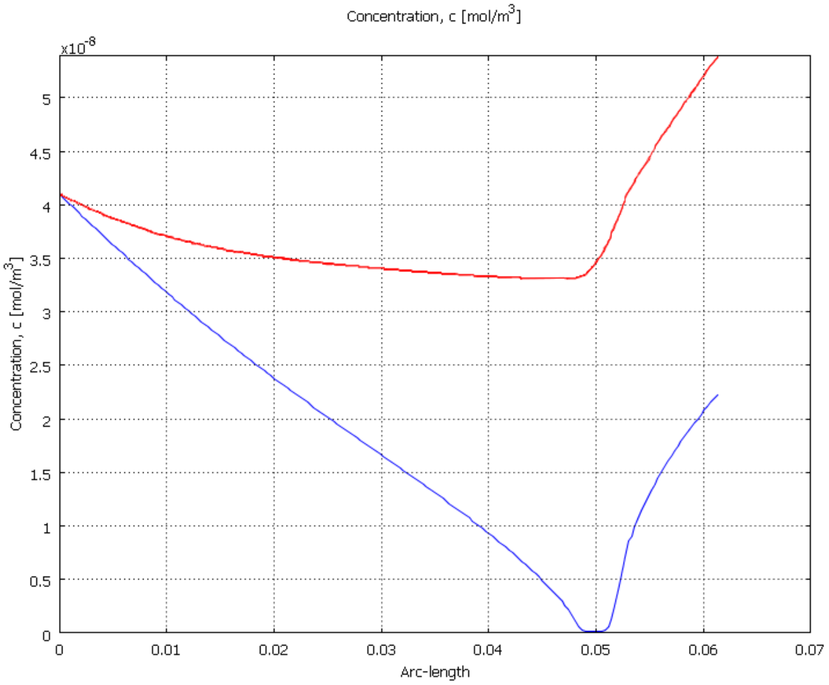


Fig. 3: Concentration contours over the length of the lens during overnight wear of regular hydrogel (red) and silicone hydrogel (blue) in mol/cm^3.

These low oxygen concentrations of the silicone hydrogel were not expected, based on the marketing claim. It was expected that although the hydrogel might perform better in day use, the silicone hydrogel would provide a higher oxygen concentration in the stroma during overnight wear. These unexpected results might be due to the boundary condition at the surface of the contact lens. This condition was largely due to the water content in the lens, as the conversion was based on Henry's law calculations with the atmosphere. Since the silicone hydrogel had a much lower percent water content, its boundary condition was much lower, as previously discussed. As a result of this low oxygen boundary condition, the high diffusivity of the silicone hydrogel was unable to overcome this obstacle. Diffusivity in silicone hydrogels is limited by water content, while water content is the basis increasing diffusivity in hydrogels [Efron, *et al*]. When keeping this contact lens boundary condition constant at 40% of 2.73 x10^{-7} mol/cm^3 (oxygen concentration in pure water), to compare the difference between the two lenses, the average oxygen concentration in the stroma, when using a silicone hydrogel, was 6.86 x10^{-8} mol/cm^3. The value when using a hydrogel lens was 6.21 x10^{-8} mol/cm^3. Clearly, with a difference of 9.9%, the difference is not substantial, but noticeable. Likewise, the silicone hydrogel *does,* in fact, exhibit a larger concentration in this case. Thus, supposing there were a way to increase the boundary condition for the silicone hydrogel lens, it would be beneficial. In its current state, however, the silicone hydrogel lacks increased oxygen concentration compared to the hydrogel.

Sensitivity Analysis:

The sensitivity analysis is done to determine which variables have the greatest effect on the results. The parameters varied in the analysis are the values of permeability Dk, therefore diffusivity D, water content W, and thickness of the contact t. The percentage of the initial concentration of oxygen is varied to model when the eye is closed. Values for the permeability, water content, and thickness are reported by the contact lens manufacturers [eyetopics.com]. Our analysis is based on the measured values and the standard deviation of these variables [Efron *et al*]. One standard deviation above and below the measured value was used to determine the sensitivity of the model to each variable. The average concentration of oxygen in the stroma was used to compare the results.

The variation in the permeability Dk of the contact lenses does not have a significant effect on the concentration of oxygen in the stroma due to the small percent error, as shown in Table 1. Only a small range was examined because the permeability is a material property and therefore cannot vary greatly. Our calculations show that we can hold the permeability constant in our model when comparing the effects of other variables.

Table 1: Sensitivity analysis for the permeability Dk of the contact lens for the average concentration in the stroma.

Contact Lens:	Focus Night and Day	
Dk [cm2-mLO2 s-mL-mm Hg]	Cavg [mol/cm3]	% Error
1.400E-09	4.198608E-08	0.15
1.522E-09	4.202442E-08	0.06
1.580E-09	4.204058E-08	0.02
1.620E-09	4.205104E-08	0.00
1.630E-09	4.205358E-08	0.01
1.718E-09	4.207467E-08	0.06

Contact Lens:	1-Day Acuvue	
Dk [cm2-mLO2 s-mL-mm Hg]	Cavg [mol/cm3]	% Error
2.00E-10	9.048875E-08	0.41
2.05E-10	9.067938E-08	0.20
2.08E-10	9.078979E-08	0.08
2.10E-10	9.086183E-08	0.00
2.14E-10	9.100229E-08	0.15
2.20E-10	9.120433E-08	0.38

Based on our analysis, thickness has very little effect on the diffusivity of oxygen through the contact lens. The calculations for the hydrogel 1-Day Acuvue show that there is only 3.81% error (Table 2) when the thickness of the contact is reduced from 118 µm to 80 µm or by 32%. Based on this information we were able to hold the thickness of both contact lenses constant for our model.

Table 2: Sensitivity analysis for the thickeness of the contact lens for the average concentration in the stroma.

Contact Lens:	Focus Night and Day	
Thickness [um]	Cavg [mol/cm3]	% Error
70	4.204592E-08	0.14
73	4.202796E-08	0.10
76	4.201000E-08	0.06
79	4.199208E-08	0.01
80	4.198608E-08	0.00
82	4.197421E-08	0.03

Contact Lens:	1-Day Acuvue	
Thickness [um]	Cavg [mol/cm3]	% Error
80	9.100229E-08	3.81
100	8.920425E-08	1.76
114	8.800104E-08	0.38
116	8.783288E-08	0.19
118	8.766558E-08	0.00
120	8.749925E-08	0.19
122	8.733379E-08	0.38

The sensitivity analysis shows that water content has a greater effect on the diffusivity of the silicone hydrogel compared to the hydrogel lenses due to the higher percent error, as shown in Table 3. The silicone hydrogel lenses are more sensitive to water content because water content is the limiting factor. Oxygen moves through the silicone material easier than it does through water [Efron *et al*]. In hydrogel contact lenses the water content is the main factor of oxygen diffusivity because oxygen travels through the water to reach the surface of the cornea.

Table 3: Sensitivity analysis of the water content in the contact lens for the average concentration in the stroma.

Contact Lens:	Focus Night and Day	
Water Content	Cavg [mol/cm3]	% Error
0.198	3.496875E-08	13.3
0.21	3.698910E-08	8.3
0.23	4.032700E-08	0.0
0.24	4.198608E-08	4.1
0.25	4.364042E-08	8.2
0.262	4.562079E-08	13.1

Contact Lens:	1-Day Acuvue	
Water Content	Cavg [mol/cm3]	% Error
0.54	8.508442E-08	6.5
0.56	8.804804E-08	3.2
0.58	9.100229E-08	0.0
0.6	9.394713E-08	3.2
0.63	9.834650E-08	8.1
0.65	1.012674E-07	11.3

Conclusion and Design Recommendations:

In both night and day conditions, the hydrogel contact lenses resulted in higher oxygen concentrations than silicone hydrogel ones. Even though the high oxygen diffusivity of silicone hydrogel made it seem like it would let more oxygen into the cornea, its low water content had a greater effect on the low oxygen concentration in the end.

From the knowledge we have gained through these simulations, it is clear that the concept of a silicone hydrogel is advantageous, yet not currently implemented with great success. The low water content and high diffusivity attributes make it ideal for passing oxygen through the material, but the lens is unable to absorb a lot of oxygen from the atmosphere. A hydrogel lens may perform slightly worse in comparison with a silicone hydrogel given equal boundary conditions. However, its ability to absorb more oxygen from the atmosphere makes it an overall more versatile lens.

While there was much consideration on the values chosen to be implemented in the simulation, much of the data was derived from scientific writing and general knowledge. Through unit conversions it is possible that accuracy was lost. Similarly, it is possible that silicone, itself, is able to accept a noticeable amount of oxygen from the atmosphere. It is advisable that more experimentation be done to get possible values directly, rather than through calculating by formulae.

Adding an ultrathin layer of a material with high water content material, such as a hydrogel, to a silicone hydrogel, it may be possible to increase the boundary condition of the lens substantially without decreasing the functionality of the silicone hydrogel by much. This fusion of two materials and layers is likely difficult to mass-produce and will be costly. In theory, this would not disrupt function, but another approach involving only one material or layer might be more successful in practice.

While development of a contact lens with a new material displaying properties of high oxygen absorbance *and* oxygen diffusion may seem costly or time consuming, it is likely to pay off economically and be easier to manufacture. The simple implementation of such a device, assuming it contains no poisonous materials would improve health and safety, as the purpose of the change is to increase oxygen flow into the cornea, thereby decreasing irritation and swelling.

Another possibility that might be more successful in the short run is altering the matrix of the silicone hydrogel to hold a higher water content. This would allow for more oxygen absorption into the contact, while affecting the diffusivity minimally. Ultimately, in this case, minor increases in water content greatly improve the boundary condition, while diffusivity is barely decreased. Again, this would be relatively easy to manufacture, with little additional up-front cost, while the health benefits are immense.

Appendix A

Governing Equation:

Mass species equation with transient, diffusion, and degradation terms:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - R_A$$

Initial and Boundary conditions:

Below shows the calculations leading to the initial conditions and boundary conditions shown previously. The final computations are not included here, as they are dependent on water content.

Eye is Open

For lens: $C(t=0) = W*pO_2 = W*0.21 * 1\text{atm} / 769.23\ [\text{atm} / M] = W*.000273\ M = W*2.73*10^{-7}\ \text{mol} / \text{cm}^3$

For cornea: $C(t=0) = W*2.73*10^{-7}\ \text{mol/cm}^3$

$C(x=0)=W *2.73*10^{-7}\ \text{mol/cm}^3$

$C(x=.0613)=C_{min} = (24\ \text{mmHg} / 760\ \text{mmHg/atm}) * 1\ \text{atm} / 769.23\ [\text{atm}/M] = 4.105*10^{-8}\ \text{mol/cm}^3$

*Where W is the water content of the contact lens.

For all side (top / bottom of schematic) and interior boundaries, assume flux = 0.

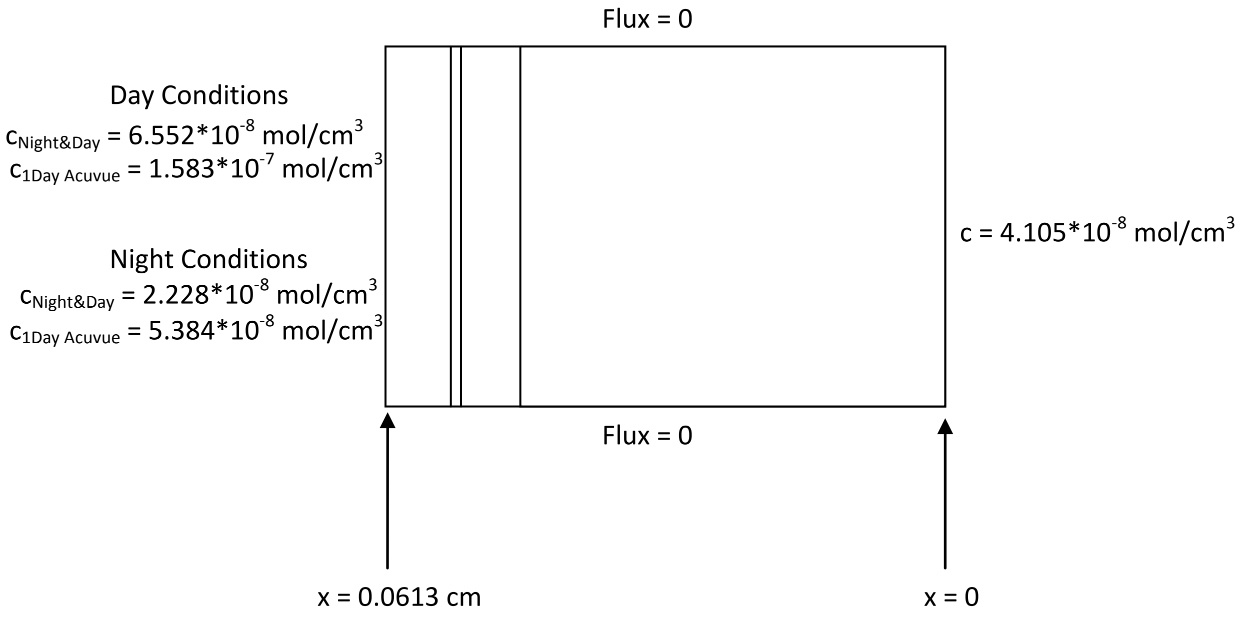
Eye is closed

All conditions are the same as above except c(x=0).

$C(x=0)=0.34*W*2.73*10^{-7}\ \text{mol/cm}^3=W * 9.28*10^{-8}\ \text{mol/cm}^3$

*Again, W is the water content of the contact lens.

When the eye is closed the initial concentration at the surface of the contact is 34% of the concentration when the eye is opened [Brennan, A Model].



Input Parameters:			
Region	D [cm2/s]	W	R [mol/cm3-s]
Contact Lens:			
Night & Day	3.19E-03	0.24	
1Day Acuvue	2.02E-04	0.58	
Tear Layer	4.27E-04	1	
Epithelium	1.20E-04	0.86	-1.16E-11
Stroma	1.09E-04	0.86	-1.02E-12
Other Constants			
kw [mgO2/LH2O]	0.404595		
rho [mg/mL]	1.42		
H [atm/M]	769.23		

The contact lens specifications are from eyetopics.com, the eye information is from Brennan's article Beyond Flux and the Kw value is from Ji.

Table 4: Results for the closed eye simulation using the average concentration in the stroma and c is the ratio to the eye open condition. For example c=0.1 represents 10% of the oxygen at the surface of the contact lens when the eye is opened.

Contact Lens:	Focus Night and Day	
Consider c as a ratio to eye open condition		
c	Cavg [mol/cm3]	% Error
1.00	4.198608E-08	98.1
0.80	3.470526E-08	63.7
0.55	2.651919E-08	25.1
0.45	2.352703E-08	11.0
0.40	2.233055E-08	5.34
0.35	2.119774E-08	0.00
0.30	2.090108E-08	1.40
0.25	2.069603E-08	2.37
0.10	2.048223E-08	3.38

Contact Lens:	1 Day Acuvue	
Consider c as a ratio to eye open condition		
c	Cavg [mol/cm3]	% Error
1.00	9.100229E-08	157
0.80	7.267504E-08	106
0.55	5.088796E-08	43.9
0.45	4.301008E-08	21.6
0.40	3.937584E-08	11.3
0.35	3.536442E-08	0.00
0.30	3.294567E-08	6.84
0.25	3.027339E-08	14.4
0.10	2.637002E-08	25.4

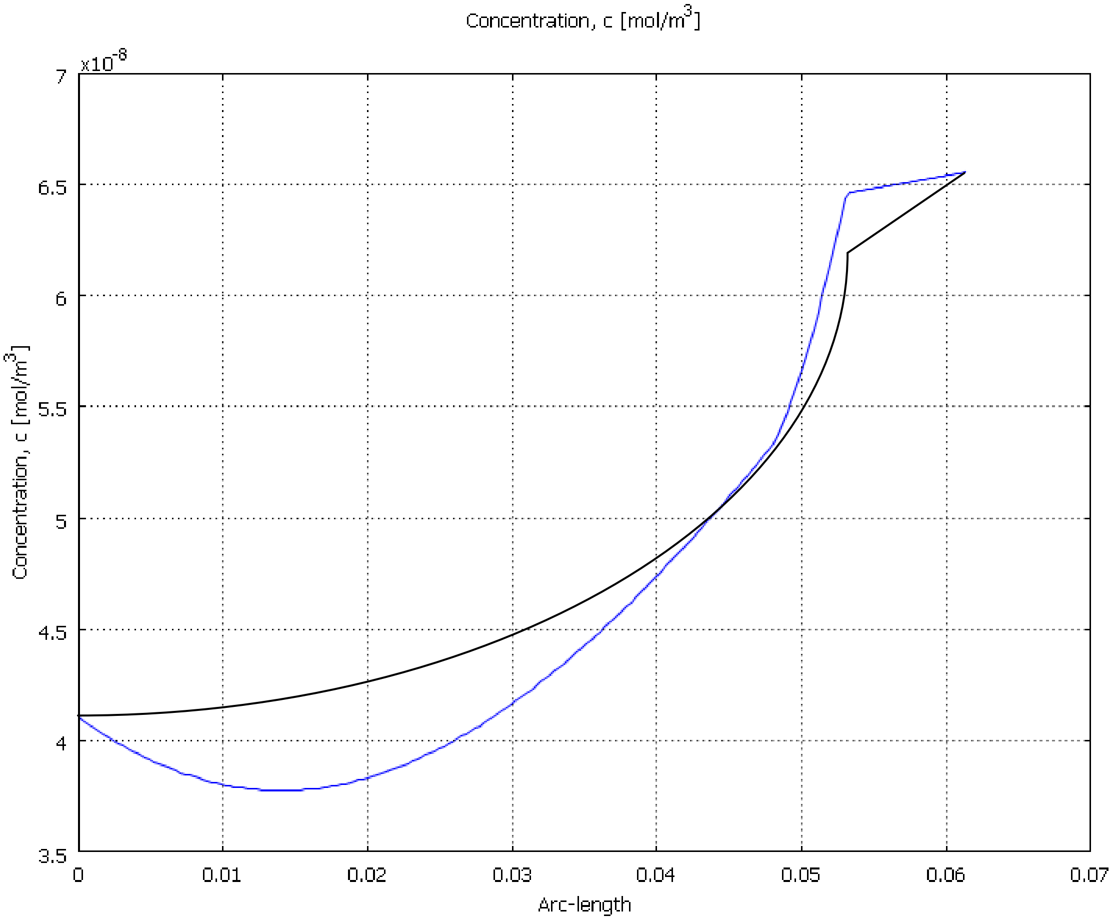


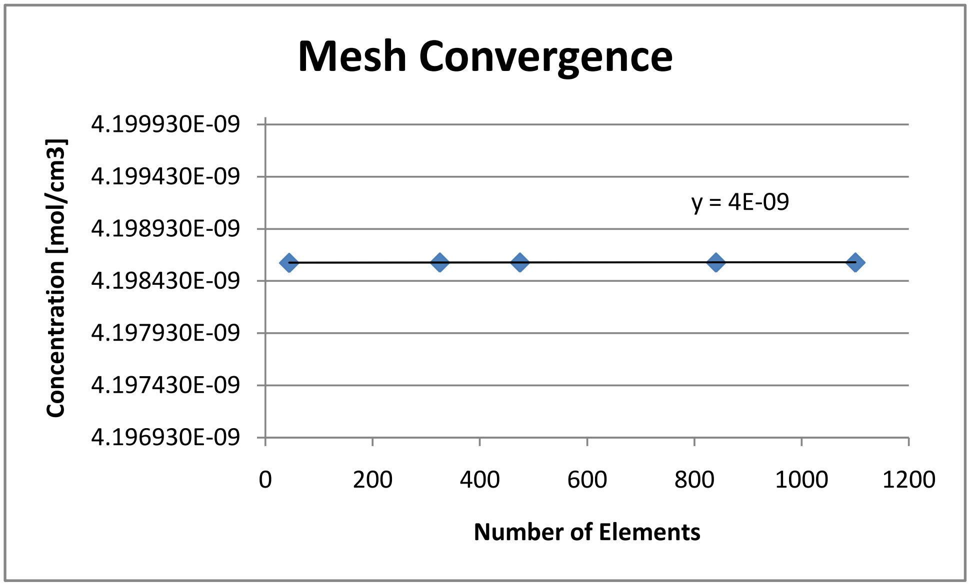
Fig. 4: Simulated concentration of silicone hydrogel during the day, compared to general curve of experimental results

Mesh Convergence

The average temperature in the stroma was used to determine if the results were sensitive to the number of mesh elements. The range of elements from 325 to 5,900 shows no difference in temperature. The only difference we found was when using only 44 elements and even then the difference in concentration was 1x10^{-16}. During our tests we used 475 mesh elements.

Table 5: Mesh convergence analysis for the average concentration in the stroma.

Number of Elements	Concentration [mol/cm3]
44	4.198604E-09
325	4.198608E-09
475	4.198608E-09
840	4.198608E-09
1100	4.198608E-09
5900	4.198608E-09


Mesh Convergence
Concentration [mol/cm3]
4.199930E-09
4.199430E-09
4.198930E-09
4.198430E-09
4.197930E-09
4.197430E-09
4.196930E-09
y = 4E-09
0
200
400
600
800
1000
1200
Number of Elements

Special conditions:

The specifications for contact lenses are given in terms of permeability, denoted Dk, where D is diffusivity and k is solubility. In order to implement our model in COMSOL we needed to calculate the diffusivity D from permeability Dk. We found a paper that defines k where k=k_w*W, where k_w is the solubility of oxygen in water and W is the water content as a percentage [Beruto]. The values for k_w is temperature dependent [Ji *et al.*]. The temperature we used was 25^{o}C because the contact will be closer to room temperature than the body's core temperature. The diffusivity is also dependent on the partial pressure of oxygen at the location. We assumed the water content of the cornea to be 86% and constant throughout the epithelium and stroma [Pircher, *et al.*]. The Dk values and the water content for Focus Day and Night Contact Lenses (Silicone hydrogel) and 1-Day Acuvue (hydrogel) were used to calculate the diffusivity for each lens [eyetopics.com].

We were unable to find oxygen consumption rates for the cornea, the only information we could was for oxygen consumption rates Q. We converted oxygen consumption rates Q into oxygen degradation rates r [Brennan, Beyond Flux]. The oxygen consumption rates are based on the measured amount of oxygen consumed in a certain volume for unit time. Therefore the consumptions rates give an average of the oxygen consumed. When we converted the consumption rates to degradation rates r a zero order reaction is assumed.

Sample Calculations:
Diffusion coefficient D from permeability Dk:

$$D = \frac{Dk \cdot \rho \cdot P}{K_w \cdot W}$$

D: Diffusion Coefficient
Dk: Permeability
ρ: density
K_w: solubility of water
W: water content (%)
P: pressure at location

$$D = \frac{\left(140x10^{-11} \frac{cm^2 \cdot mL_{O2}}{s \cdot mL \cdot mmHg}\right) \cdot \left(1.429 \frac{mg_{O2}}{mL}\right) \cdot (155\ mmHg) \cdot \left(1000 \frac{mL}{L}\right)}{\left(0.404595\ \frac{mg_{O2}}{L}\right) \cdot (0.24)}$$

$$D = 3.19x10^{-3}\ \frac{cm^2}{s}$$

Degradation Rate r:

R = Q·ρ·MW
Q: Oxygen consumption
ρ: Density
MW: Molecular weight

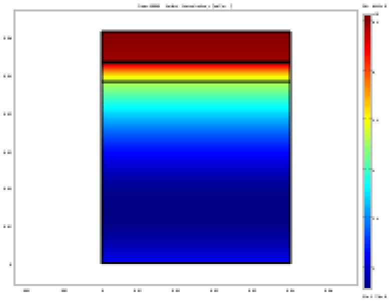
$$R = \left(-47.78x10^{-5}\ \frac{\mu L}{cm^3 \cdot s}\right) \cdot \left(10^{-6}\ \frac{L}{\mu L}\right) \cdot \left(1.49\ \frac{g}{L}\right) \cdot \left(\frac{1\ mol}{32\ g}\right)$$

$$R = -2.124x10^{-11}\ \frac{mol}{cm^3 \cdot s}$$

While doing sensitivity analysis for the closed eye condition we ran into problems because concentration of oxygen in the stroma became negative, which is not physically possible. To resolve this problem we added a function in COMSOL what would only use a degradation rate when the concentration of oxygen is greater than zero. This function also gave us problems. The problems were finally solved by adding a smoothing function to the degradation rate. The smoothing function causes the computer to think the concentration is zero when the concentration is $1x10^{-9}$ mol/cm^3. The value of the $1x10^{-9}$ mol/cm^3 was chosen because it is two orders of magnitude smaller than the concentrations we are dealing with, therefore will not affect the results. When the computer believes the concentration is zero the degradation rate is smoothed to zero. This function prevents there from being sharp drop from the degradation rate to zero.

Appendix B:

COMSOL Model Report



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2. Model Properties

Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Apr 8, 2008 5:02:18 PM
Creation date	Feb 14, 2008 8:36:34 PM
COMSOL version	COMSOL 3.3.0.511

File name: C:\Documents and Settings\labuser\Desktop\preliminary_work.mph
Application modes and modules used in this model:
Geom1 (2D)
Diffusion

3. Constants

Name	Expression	Value	Description
Kw	.404595		Water solubility (mgO2)
rho	1.429		Density (mg/mL)
H	584614.8		Henry's Law Constant (mmHg L/mol)

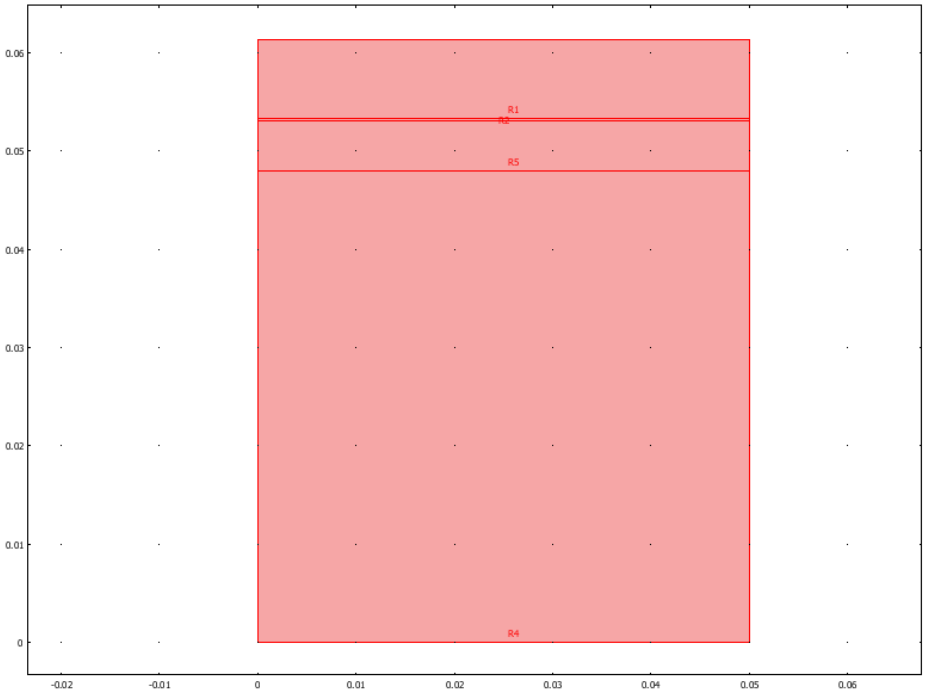
4. Global Expressions

Name	Expression	Description	
D	(1000*rho*H) / (Kw)		

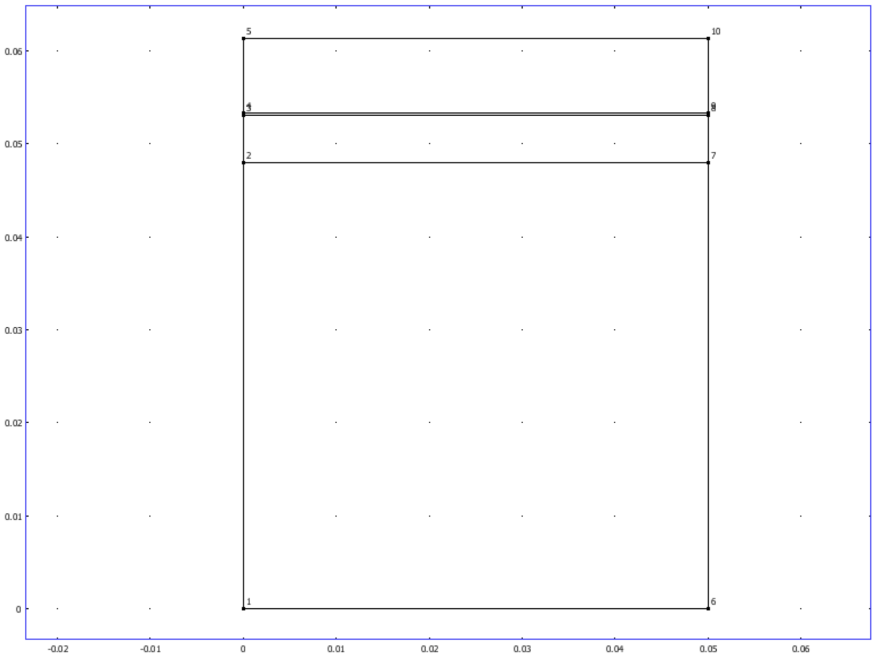
5. Geometry

Number of geometries: 1

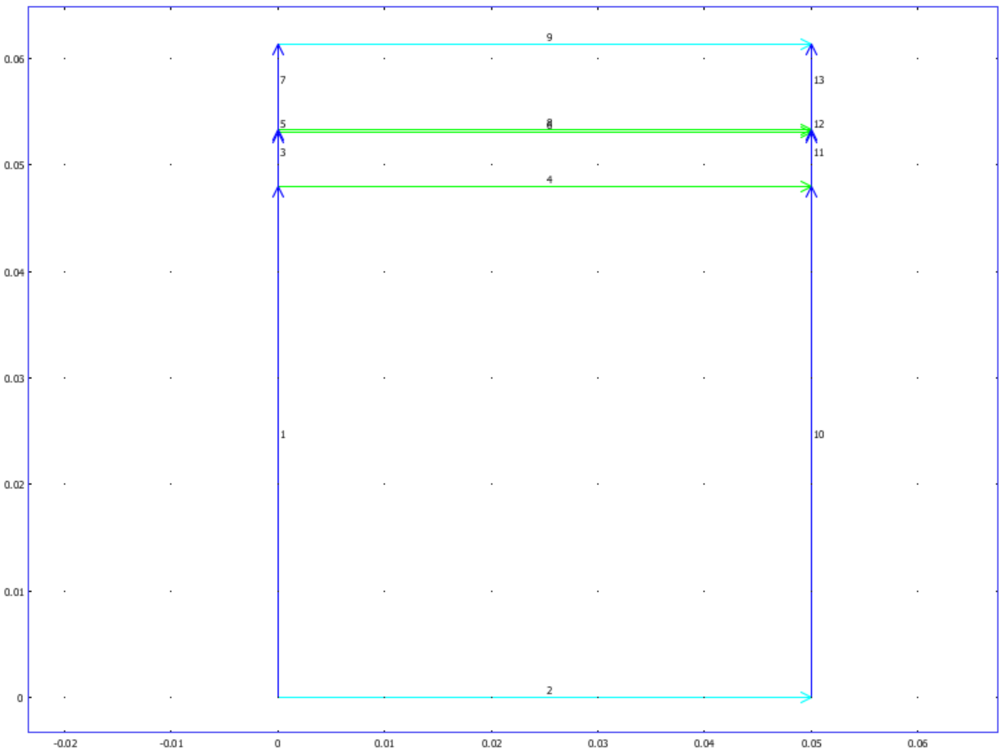
5.1. Geom1



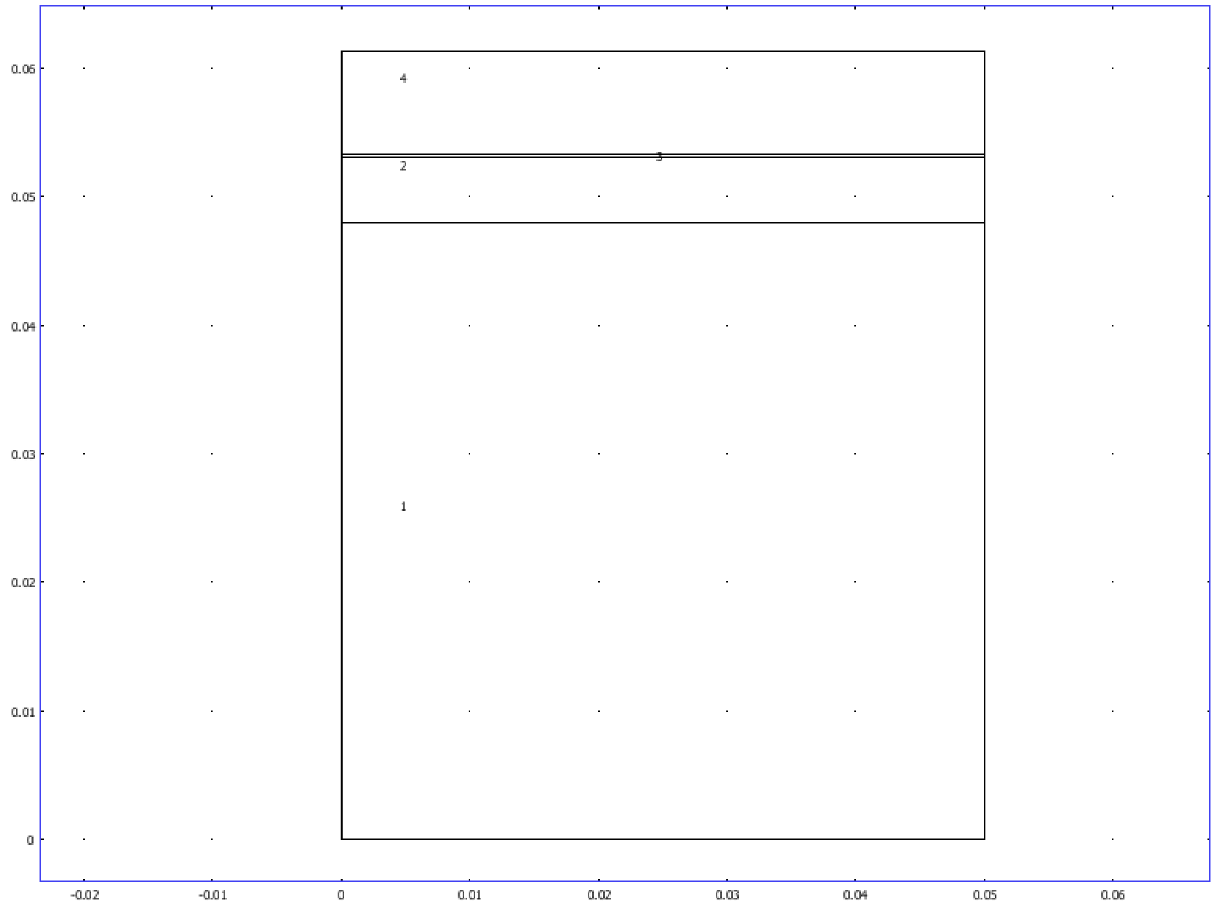
5.1.1. Point mode



5.1.2. Boundary mode



5.1.3. Subdomain mode



6. Geom1

Space dimensions: 2D

Independent variables: x, y, z

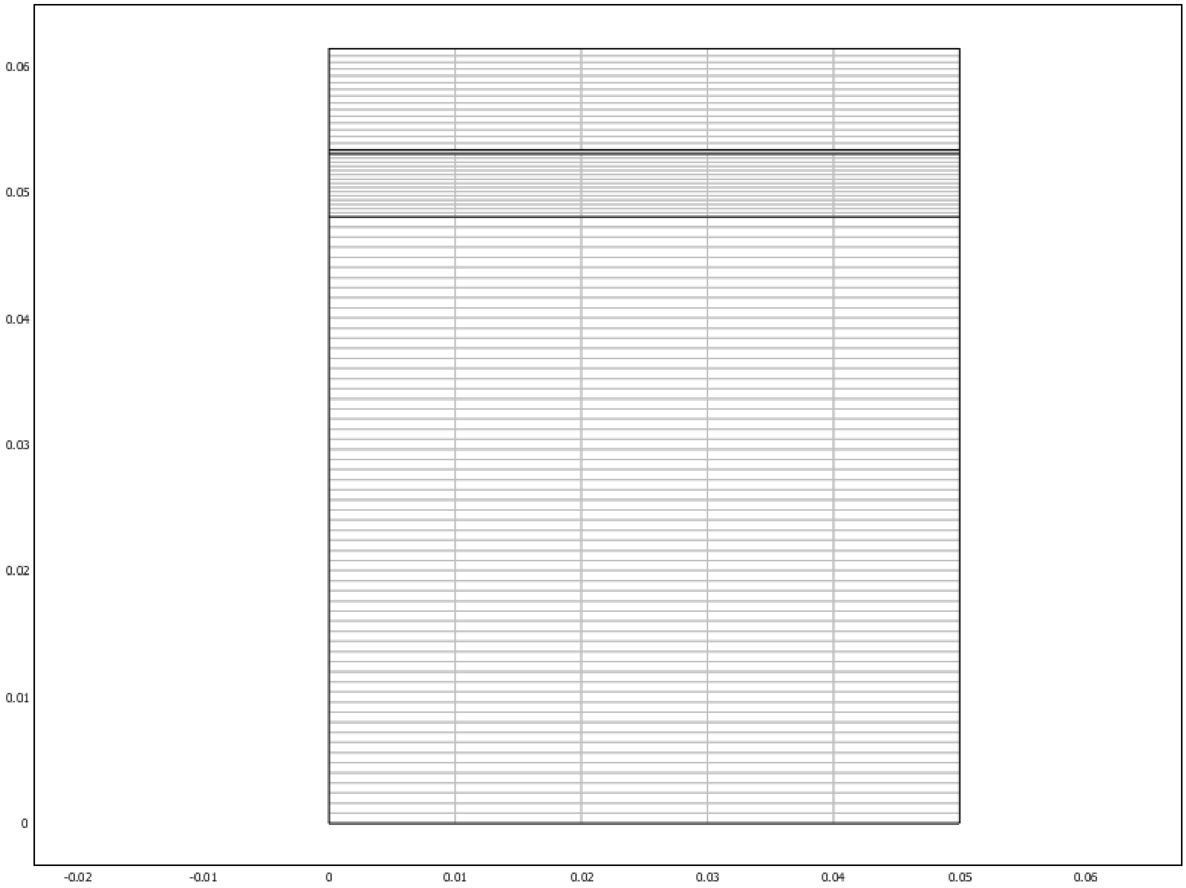
6.1. Scalar Expressions

Name	Expression
sqwv	sign(sin(2*pi*t/6)+.998)

6.2. Mesh

6.2.1. Mesh Statistics

Number of degrees of freedom	2101
Number of mesh points	576
Number of elements	475
Triangular	0
Quadrilateral	475
Number of boundary elements	215
Number of vertex elements	10
Minimum element quality	0.012
Element area ratio	0.075



6.3. Application Mode: Diffusion (di)

Application mode type: Diffusion
Application mode name: di

6.3.1. Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Analysis type	Transient
Frame	Frame (ref)
Weak constraints	Off

6.3.2. Variables

Dependent variables: c
Shape functions: shlag(2,'c')
Interior boundaries not active

6.3.3. Boundary Settings

Boundary		1, 3, 5, 7, 10-13	2
Type		Insulation/Symmetry	Concentration
Concentration (c0)	mol/m^3	0	**4.105E-8**

Boundary	9
Type	Concentration
Concentration (c0)	**2.73E-7*.24**

6.3.4. Subdomain Settings

Subdomain		1	2
Diffusion coefficient (D)	m^2/s	**D*c*29.5E-11/.86**	**D*c*18.8E-11/.86**
Reaction rate (R)	mol/(m^3·s)	**-1.023E-12*(flc2hs(c-1e-9,1e-9))**	**-1.157E-11*(flc2hs(c-1e-9,1e-9))**

Subdomain	3	4
Diffusion coefficient (D)	**D*c*78E-11/1**	**D*c*140E-11/.24**
Reaction rate (R)	0	0

Subdomain initial value		1	2	3	4
Concentration, c (c)	mol/m^3	2.73E-7*.24	2.73E-7*.24	2.73E-7*.24	2.73E-7*.24

7. Solver Settings

Solve using a script: off

Analysis type	Transient
Auto select solver	On
Solver	Time dependent
Solution form	Automatic
Symmetric	auto
Adaption	Off

7.1. Direct (UMFPACK)

Solver type: Linear system solver

Parameter	**Value**
Pivot threshold	0.1
Memory allocation factor	0.7

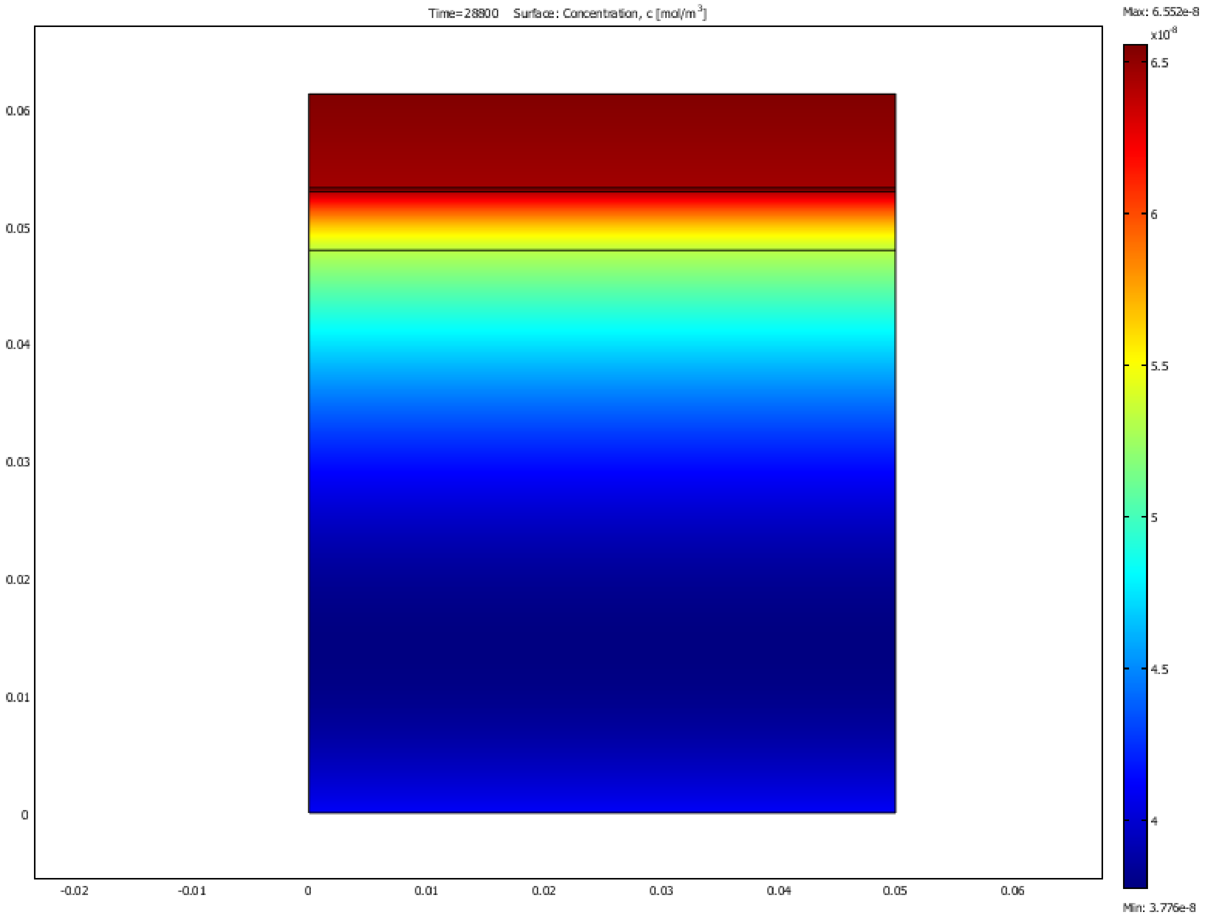
7.2. Time Stepping

Parameter	Value
Times	0:10:28800
Relative tolerance	0.01
Absolute tolerance	0.0010
Times to store in output	Specified times
Time steps taken by solver	Intermediate
Manual tuning of step size	On
Initial time step	0.0010
Maximum time step	10
Maximum BDF order	5
Singular mass matrix	Maybe
Consistent initialization of DAE systems	Backward Euler
Error estimation strategy	Include algebraic
Allow complex numbers	Off

7.3. Advanced

Parameter	Value
Constraint handling method	Elimination
Null-space function	Automatic
Assembly block size	5000
Use Hermitian transpose of constraint matrix and in symmetry detection	Off
Use complex functions with real input	Off
Stop if error due to undefined operation	On
Type of scaling	Automatic
Manual scaling	
Row equilibration	On
Manual control of reassembly	Off
Load constant	On
Constraint constant	On
Mass constant	On
Damping (mass) constant	On
Jacobian constant	On
Constraint Jacobian constant	On

8. Postprocessing



9. Variables

9.1. Boundary

Name	Description	Expression
ndflux_c_di	Normal diffusive flux, c	nx_di * dflux_c_x_di+ny_di * dflux_c_y_di

9.2. Subdomain

Name	Description	Expression
grad_c_x_di	Concentration gradient, c, x component	cx
dflux_c_x_di	Diffusive flux, c, x component	-Dxx_c_di * cx-Dxy_c_di * cy
grad_c_y_di	Concentration gradient, c, y component	cy
dflux_c_y_di	Diffusive flux, c, y component	-Dyx_c_di * cx-Dyy_c_di * cy
grad_c_di	Concentration gradient, c	sqrt(grad_c_x_di^2+grad_c_y_di^2)
dflux_c_di	Diffusive flux, c	sqrt(dflux_c_x_di^2+dflux_c_y_di^2)

REFERENCES

1. Beruto, D.T., Botter, R. Role of the water matric potential (ψ_M) and of equilibrium water content (EWC) on the water self-diffusion coefficient and on the oxygen permeability in hydrogel contact lenses. *Biomaterials* 2004, 25:2877-2883.

2. Brennan, Noel A. Beyond Flux: Total Corneal Oxygen Consumption as an Index of Corneal Oxygenation During Contact Lens Wear. *Optometry and Vision Science* 2005; 82 (6): 467-472.

3. Brennan, Noel A. A Model of Oxygen Flux Through Contact Lenses. *Cornea* 2001; 20 (1): 104-108.

4. Efron, Nathan, Morgan, Philip B., Cameron, Lan D., Brennan, Noel A., Goodwin, Marie. Oxygen permeability and water content of silicone hydrogel contact lens materials. *Optometry and Vision Science* 2007; 84 (4): 1040-5488.

5. Holden, Brien A., Mertz, George W. Critical Oxygen Levels to Avoid Corneal Edema for Daily and Extended Wear Contact Lenses. *Investigative Ophthalmology & Visual Science* 1984; 25: 1161-1167

6. Ji P., Feng W., Tan T., and Zheng D. Modeling of water activity, oxygen solubility, and density of sugar and sugar alcohol solutions. Food Chem 2007; 104: 551-8.

7. Pircher M., Gotzinger E., Leitgeb R., Fercher A., and Hitzenberger C. Measurement and imaging of water concentration in human cornea with differential absorption optical coherence tomography. Opt Express 2003; 11: 18

8. http://www.eyetopics.com/categories/Contact-Lenses/Contact-Lens-Reviews/ accessed January 23, 2008