Article

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Carbon Dioxide Loss of Carbonated Beverages in Pet Packaging: Experimental and Numerical Findings

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Abstract

In this study, we investigated the change of carbon dioxide (CO_2) gas in PET bottles over time using experimental and numerical methods, as this is an important quality criterion in carbonated beverage production. Gas loss was modeled using the finite element method (FEM) on 2.5-liter PET bottles, and the effects of temperature, internal pressure, and packaging wall thickness were theoretically evaluated within the framework of the ideal gas equation and Fick's law. Validation was achieved by comparing model results with experimental data, and ideal production conditions were determined. Analyses revealed that gas loss was concentrated primarily in the top and shoulder regions of the bottle, and increasing the thickness in this region reduced diffusion. Furthermore, lowering the filling temperature and increasing internal pressure significantly reduced the transfer of dissolved CO_2 from the packaging to the external environment. Modeling studies were conducted using a three-dimensional design of the bottle geometry, defining boundary conditions to investigate the effects of different material distributions and thicknesses. Based on the findings, production processes were reorganized, and standardized recipes were created. As a result, the combination of experimental and numerical data has shown that gas losses have been largely controlled, and quality standards can be maintained for longer periods. This study can provide guidance not only for 2.5-liter PET bottles but also for other packaging types. Thus, it was concluded that more planned, higher standard production can be achieved in the carbonated beverage industry, consumer complaints can be reduced, and product performance can be maintained sustainably.

Keywords: carbon dioxide; diffusion; boundary conditions; experimental and numerical analysis

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1. Introduction

The carbonated beverage industry has become a rapidly growing sector on a global scale due to the increasing population and changing dietary habits (Teenand & Ashurts, 2006). Cola drinks, fruit-flavored carbonated drinks, and soda-like products constitute the main product groups in this industry (Steenand & Ashurst, 2006; Ashurst, 2005). Recently, efforts to reduce quality-related problems and increase customer satisfaction have gained significant importance, and in parallel, improvement efforts in production processes have accelerated (Ashurst, 2005). Today, carbonated beverage consumption is estimated to have reached 3.3 billion liters, with high growth potential particularly evident in regions such as the United States, Northern Europe, Mexico, Eastern Europe, and China (Steenand & Ashurts, 2006). The main reason for the dominance of cola drinks in the American market is that the two leading companies of the sector were established in this region. While cola drinks account for approximately half of total soda consumption in Europe and Japan, this share reaches 70% in the United States (Steenand & Ashurst, 2006; Ashurst, 2005). While the average annual per capita consumption in European countries is 82 liters, this amount is around 45 liters in Turkey, indicating that the sector has a lower development potential compared to other countries (Ashurst, 2005).

One of the most important components of carbonated beverages is carbon dioxide. Carbon dioxide is widely used in the food and beverage industry; its refreshing mouthfeel and digestive properties directly influence drinking preferences (Nigar, 2005; Shahman, 2005). Furthermore, carbon dioxide imparts a unique flavor to beverages and increases product safety by inhibiting microbial growth (Çakır, 2010). To be defined as a carbonated beverage, the carbon dioxide level must be at least 2 g/L (Nigar, 2005). However, the amount of carbonated beverages used varies depending on the product type and the manufacturer's formulation preferences (Steenand & Ashursts, 2006; Ashurst, 2005).

In the production of carbonated beverages, carbon dioxide solubility in water is determined by parameters such as temperature and pressure. Studies conducted by Krones UK clearly demonstrated the effects of temperature and pressure variables on solubility (Steenand & Ashurts, 2006). When examining the components of carbonated beverages, it is seen that more than 85% of the total content is water (Ashurst, 2005).

Studies on carbon dioxide loss in carbonated beverages stored in PET bottles indicate that the properties of the polymer structure, storage temperature, and bottle wall thickness have significant effects (Çakır, 2010). David and colleagues (Steenand & Ashurts, 2006) and Lewis and colleagues (Lewis et al., 2003) investigated the barrier properties of the PET polymer structure and the role of temperature on the stability of dissolved gas. Similarly, Chanda and Roy (2007) investigated the effects of storage conditions and material distribution on shelf life. Del et al. (1997) compared the gas loss in PET bottles with experimental data using the mathematical model they developed and revealed a strong relationship between bottle wall thickness and gas loss.

This study examined the time-dependent change in dissolved carbon dioxide in carbonated beverages stored in PET bottles. By optimizing production parameters like filling pressure, product temperature, and bottle material distribution, the study sought to reduce gas loss and identify optimal production conditions. It is anticipated that the results will contribute to both increasing production efficiency and maintaining product quality. Carbonated beverages include cola and fruit-flavored drinks that are aerated with carbon dioxide gas. While their general structure is largely water, they also contain sugar or artificial sweeteners, coloring agents, flavorings, chemical preservatives such as benzoic acid and sorbic acid, and carbon dioxide gas, which imparts the beverage its unique flavor. The water used in beverages is of significant importance, depending on the proportion used. It is only possible to have the same taste in all products produced at different points with standard water. For this reason, efforts are being made to standardize all values by establishing water processing centers with large investments in production facilities. In 2015, the US drank an average of 200 liters of sparkling drinks per person, while Europe drank 90 liters and Turkey drank about 45 liters. This added up to more than 3.5 billion liters a year. It is clear that small improvements in the carbonated beverage market in Türkiye, where 37% of beverage consumption is carbonated, will have a bigger effect over time, since the market grows by 10% to 15% every year. The sparkling beverage industry has recently seen a big increase in the number of different products available, and research and development on the types of packaging used in this industry has sped up. In this regard, companies are spending a lot of money on other ways to keep product quality standards high for longer periods of time and make things cheaper.

The type of packaging in the carbonated beverage industry has varied greatly over time, especially since production costs are crucial. In the past, glass and tin can packaging were predominantly used in the sparkling beverage industry, but over time, PET bottles have largely replaced the packaging type, and due to their ease of production, various sizes have also increased. The fragile structure and difficulty of production of the glass bottle, the high production cost of the tin can, and the lack of packaging variety are significant disadvantages and are the main reason why it is less preferred in the industry. In addition to all this, PET packaging also has disadvantages that are of great importance for the carbonated beverage industry due to its physical structure. The carbon

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dioxide gas contained in sparkling beverages in PET bottles changes over time more than in glass and tin cans.

Considering the material cost and lightness, the packaging properties of 2.5 liter PET bottles used for carbonated drinks were selected as the subject of this study, and numerical and experimental data were obtained. Using the data obtained, new production conditions were defined to reduce CO_2 gas evolution within PET bottles over time. The effects of temperature, pressure, and packaging characteristics on the reduction of carbon dioxide gas over time were individually evaluated, and ideal production conditions were established.

The amount of carbon dioxide in carbonated drinks varies depending on the type of drink. To make sure that carbonated drinks are dosed correctly, manufacturers must find the best balance of temperature and pressure that affects the dosing process within the limits set by the product type. This definition makes it easy to keep an eye on and change the carbon dioxide limit that manufacturers set when they make the product. Figure 1 shows that many companies use the maximum amount of carbon dioxide that can be dissolved in water as a reference. This is because a lot of carbonated drinks are made up of water. The effect of temperature and pressure on the amount of carbon dioxide dissolved in water is also shown.To achieve the desired limits, the amount of dissolved carbon dioxide gas per unit can be increased with high pressure and low temperature by carrying out the management process in a delicate balance.

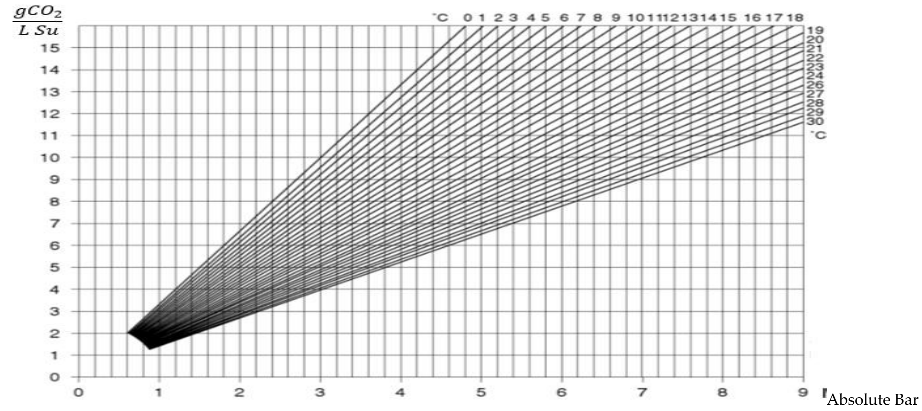

Figure 1. Solubility of carbon dioxide gas in water.

Many evaluations have helped companies in the carbonated beverage business, which is a big business. Figure 2 shows how gas loss in PET bottles changes over time (Steen & Ashurst, 2006). It also shows how gas loss is spread out at a constant temperature. The change in CO2 gas over time for different material types is shown. As can be seen in Figure 1, while the general trend is the same for different bottle types, CO2 values fluctuate based on measurements taken from different weeks. However, CO2 losses from poly materials showed a smooth decrease over time, with losses being slower in poly(Amb).

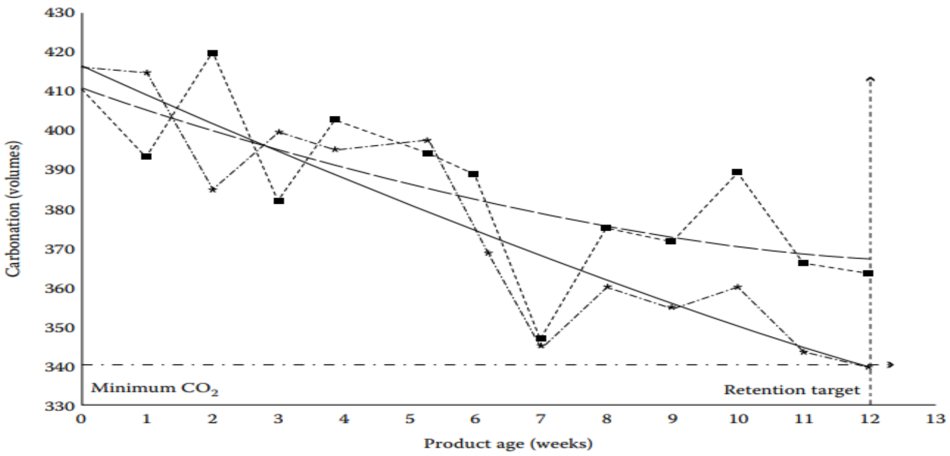

Figure 2. Carbonation loss from PET bottles. Bottles held under ambient storage conditions typical for soft drinks (--------). Bottles were held at 20°C and then chilled to 5°C for 24 hr prior to carbonation measurement (-.-.-*-.-.-). Trend line for bottles held under ambient storage conditions (— — —). The trend line represents bottles that were stored at 20°C and then chilled to 5°C for 24 hours before carbonation measurement (———). (This information is redrawn from Syrett D. 2006, which discusses bottle design and manufacture as well as related packaging.) In: Carbonated Soft Drinks Formulation and Manufacture. Steen D.P., Ashurst P.R. (Eds). Blackwell Publishing, Oxford, pp. 181–217, with permission.).

1.1. Carbonated Beverages and CO_2 Retention

Carbon dioxide is an important part of carbonated drinks because it gives them their unique taste and keeps them safe from germs. The amount of dissolved CO_2 in the product has a direct effect on how fresh it is, how good it tastes, and how long it lasts. But once the CO_2 is trapped in PET containers, some of it slowly moves through the polymer matrix and into the air around it. How well the diffusion works depends a lot on the temperature, pressure, and the properties of the PET material barrier.

Some of the CO_2 stays in the liquid phase, but some of it is in the space above the bottle cap. The loss of CO_2 could cause the internal pressure to drop slowly, which could have a big effect on quality. It's important to know how CO_2 spreads in PET bottles and how to model its behavior over time in order to predict how long a product will last and make packaging work better.

1.2. PET Packaging in Carbonated Beverages

PET bottles are the most popular choice for carbonated drinks because they are inexpensive, light, clear, and strong enough. PET is a type of polyester that can be either amorphous or semi-crystalline. It can be recycled and is very resistant to chemicals. These traits make PET great for making a lot of drink containers at once.

First, PET granules are shaped into preforms. Then, they are turned into bottles using a blow-molding process that controls the heat and pressure. The bottles that come out of this process have good dimensional stability and can handle mechanical loads well enough to be safely used in pressurized carbonated drinks.

1.3. Filling System and CO_2 Retention

The filling process is important for making sure that drinks have the right amount of dissolved CO_2. To stop the foaming, CO_2 is used to put pressure on the bottles first. Then, liquid is added in a way that keeps gas from getting out. Some of the CO_2 stays dissolved in the drink after the cap is put on, and a little bit stays in the space between the cap and the drink. Over time, CO_2 slowly gets through the PET barrier. This lowers the pressure inside and changes how things taste.

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The length of time that carbonated drinks last is directly related to how well PET bottles keep gas from getting in. To make sure the product is of good quality and to design containers, it's important to know what affects CO_2 diffusion during storage.

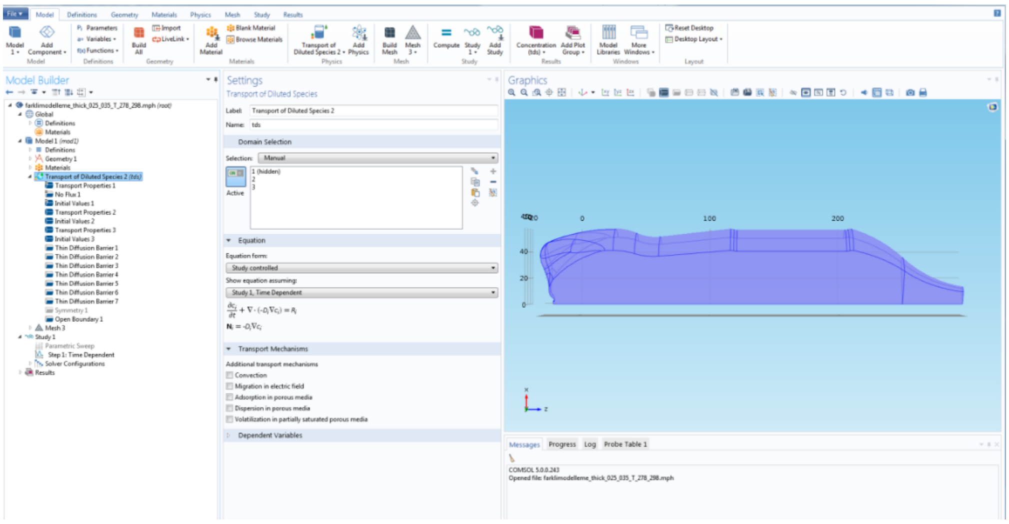
2. Solid Modeling and Numerical Analysis Assessments

2.1. Solid Model Design of the PET Bottle

A 3D solid model will be created for a 2.5 L PET bottle based on the material distribution of the bottle produced under current conditions. This design includes three separate assembly elements: the PET bottle, the liquid section, and the cushioning pressure section. These elements will be verified through a combined assembly conformity examination using a solid design program. The first step of the design process will be completed by transferring the obtained file with the step extension to the finite element program. Each element will be introduced individually in the finite element program, completing the necessary preparations for physical modeling. Design variables in the finite element interface will be introduced so that they can be used as functions. In this way, it will be possible to apply variables and observe the results without logging into the solid modeling program.

2.2. Defining Variables in the Finite Element Analysis Program

The effect of regional material distribution on the time course of CO_2 gas can be analyzed by defining different thicknesses for the regions defined by the "Thin Diffusion Barrier" in the "Transport of Diluted Species" physics model within the finite element program. Comsol software can handle these variables parametrically and display their interrelationships. In Figure 7, all regional boundary conditions are defined, allowing for functional analysis of the variables. The material distribution on the bottle will be analyzed by evaluating four different regions, and a thickness variable will be defined for the point where the total molar change is greater. Defining boundary conditions as variables will allow for obtaining results with different values.



Label: Transport of Diluted Species 2
Name: tds

Domain Selection
Selection: Manual
Active
1 (hidden)
2
3

Equation
Equation form: Study controlled
Show equation assuming: Study 1, Time Dependent

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

$$\mathbf{N}_i = -D_i \nabla c_i$$

Transport Mechanisms
Additional transport mechanisms
☐ Convection
☐ Migration in electric field
☐ Adsorption in porous media
☐ Dispersion in porous media
☐ Volatilization in partially saturated porous media

Dependent Variables

```
COMSOL 5.0.0.243
Opened file: farklimodelleme_thick_025_035_T_278_298.mph
```

Figure 7. Defining boundary conditions in COMSOL.

2.3. Numerical Analysis of Production Conditions

2.3.1. Model Creation Using Numerical Analysis

In this study, the time-dependent gas loss of 2.5 liters of cola produced under current production conditions was monitored, and analyses were conducted using the finite element method based on the obtained data. Furthermore, the mathematical model function was created using the values obtained from the experimental results and was defined in the analysis program. After seeing that the results obtained by numerical analysis were in line with the results obtained by experimental data, the optimum values of the model were adapted to the production conditions again and the reduction of time-dependent gas loss was physically achieved. Thus, improvement opportunities were identified as a reference for all bottle formats, and the effects of each variable were observed separately, and the results were examined by evaluating the best conditions identified by the model together.

2.3.2. Solid Model Design of the 2.5 L PET Bottle

The design of the 2.5 L PET bottle discussed in this study was designed using SOLIDWORKS, adhering to the available technical drawing details. The drawing was then converted to IGES format using the software's control tools, verifying all dimensions and technical values, and then transferred to the numerical analysis program. Figure 3.3 shows the 3D solid model view of the 2.5 L PET bottle, showing its complete physical structure. After the 3D solid model design was completed, the bottle was cut to 1/5 of its original size due to its symmetrical nature, simplifying the sample model as shown in Figure 8. This greatly facilitated faster numerical analysis.

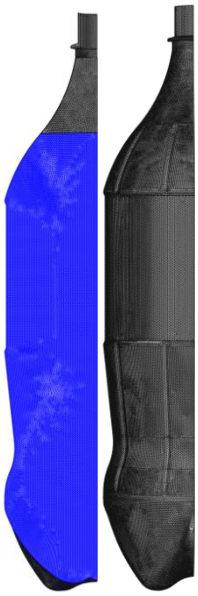


Figure 8. PET bottle 1/5 symmetrical part representation.

2.3.3. Analysis with the Finite Element Method

After the solid model was successfully created, it was imported into the finite element program to establish the necessary conditions for the analysis. Initially, the design assembly, consisting of four separate sections: the Cola, the Upper Cushioning Area, the PET Bottle, and the External Atmosphere, was defined. Immediately following the section definitions, the mesh structure of the solid model was created, and precise distribution was captured.

A tetrahedral cell-type network was created using the network creation interface within the software, and the technical details are listed in Table 6, and the general network distribution is shown in Figure 9.

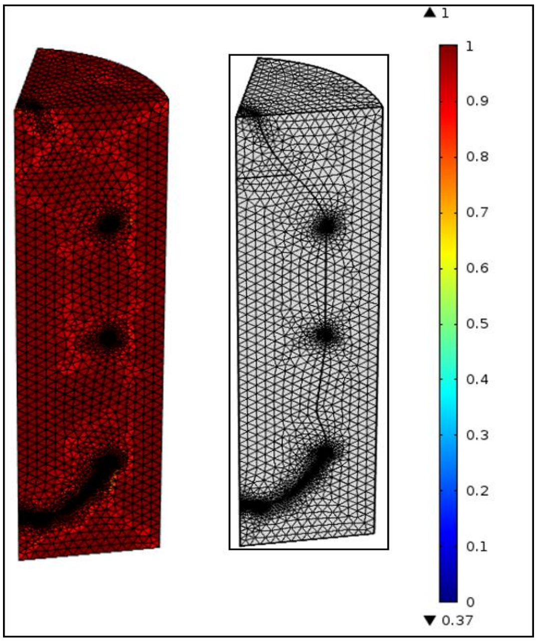


Figure 9. Structural network analysis of a 2.5 L PET bottle.

Table 6. 2.5 L 1/5 symmetrical part structural network analysis data.

Total Number of Tetrahedral Elements	*518574*
Number of Triangular Elements	*30145*
Number of Corner Elements	*2324*
Number of Top Elements	*124*
Minimum Element Quality	*0.1357*
Average Element Quality	*0.738*

In such analyses, selecting an element that can accurately represent the volume occupied by the geometry is crucial for the analysis's accuracy. The interior surface geometry of the air contained within the outer surface shares similar characteristics with the exterior surface geometry of a PET bottle. Due to the relatively narrow areas on these surfaces, the selected element structure was tetrahedral. This will enable a more accurate depiction of every area within the part and facilitate the necessary computations at the highest volume. Also, while the mesh was being applied, the element growth index was set to 1.2, and the inside of the part was made with rougher elements. The main reason for this is to speed up the calculations.

2.3.4. Defining Functions and Variables for Finite Element Numerical Analysis

The 2.5 L PET bottle we analyzed as the reference bottle was designed with exact measurements. To evaluate the current conditions, the final bottle thickness was set at l, the fluid phase volume was defined as V_1, and the cushioning region volume was defined as V_2. The fluid phase volume is in constant equilibrium with the current gas volume, and the current equilibrium is defined according to Henry's Law (Equation 3.1).

$C_{CO_2} = H.P_{co_2}$ (Equation 3.1)

C_{CO_2} is defined as the molar concentration in the cola beverage, and P_{co_2} is defined as the partial pressure value in the gas phase. H is taken as the partial constant. As soon as the internal CO_2 pressure value reaches equilibrium with the cushioning value, equality occurs within the bottle, defined as a decreasing function with time. The external atmospheric CO_2 pressure value is assumed to be 0. Total mass transfer can be calculated by evaluating the change in the CO_2 value in the fluid with time.

2.3.5. Parameter Definition for the Finite Element Numerical Analysis Program

Parameter inputs for the PET bottle, cola, and upper region are given in Tables 7–9.

Table 7. PET bottle parameter inputs.

k_d	$7{,}8354E^{-3} * \exp{(1134.3/T)}$
C_H	$13{,}252 - 1{,}7951E^4/T + 4{,}8595E^6/T^2$
b_T	$2{,}4638E^{-3} * \exp{1495{,}6/T}$
D_d	$6{,}5148E^{-6}[m^2/s] * \exp{(-4470.5/T)}$
D_H	$8{,}2863E^{-6}[m^2/s] * \exp{(-5406{,}5/T)}$
D_{eff1}	$((1 + D_H * C_H * b_t/(D_D * k_d))/\left(1 + b_t * p_{CO_2}\right)^2)$
D_{eff2}	$(1 + (C_H * b_t/k_d)/\left(1 + b_t * p_{co_2}\right)^2)$
D_{eff}	$D_d * (D_{eff1}/D_{eff2})$
P_{CO_2}	$mod1.C_2 * V_1 * 10^{-6}\,[m^3/mol]/(\frac{V_2}{Rconst * T} + H * V_1)$
H	$4{,}9976e^{-9} * \exp{(\frac{2626{,}1}{T})}$

Table 8. Parameter inputs for cola.

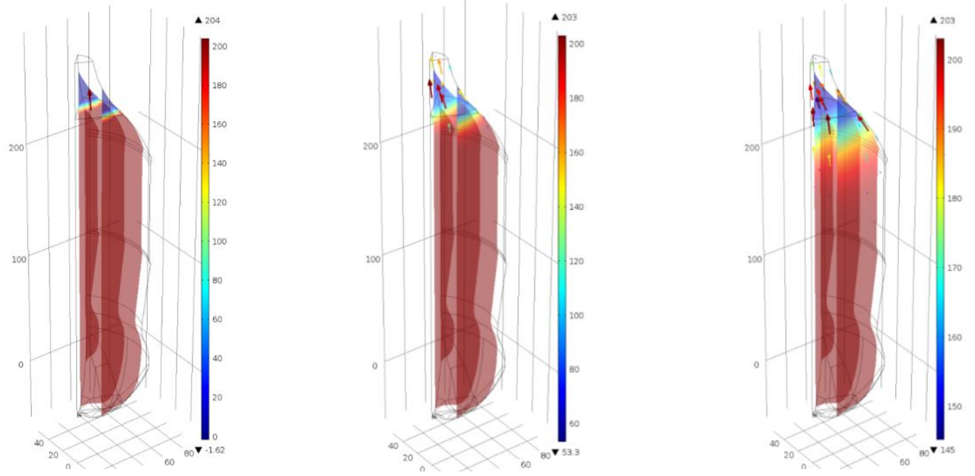
D_{Cola}	$2{,}44E^{-9}[m^2/s] * T^{1{,}5}\,\exp(-307{,}9/T) * (p_{ref}/p_{CO_2})$
CO_2	$H * p_{CO_2}$
P_{CO_2}	$mod1.C_2 * V_1 * 10^{-6}[m^3/mol]/(V_2/(R_{const} * T) + H * V_1)$
H	$4{,}9976E^{-9} * \exp(2626{,}1/T)$
P	$\exp{((1/cc) * (\log{(abs(C_2 * 1[m^3/mol]))} - a - b/T))}$

Table 9. Parameter entries for the upper part.

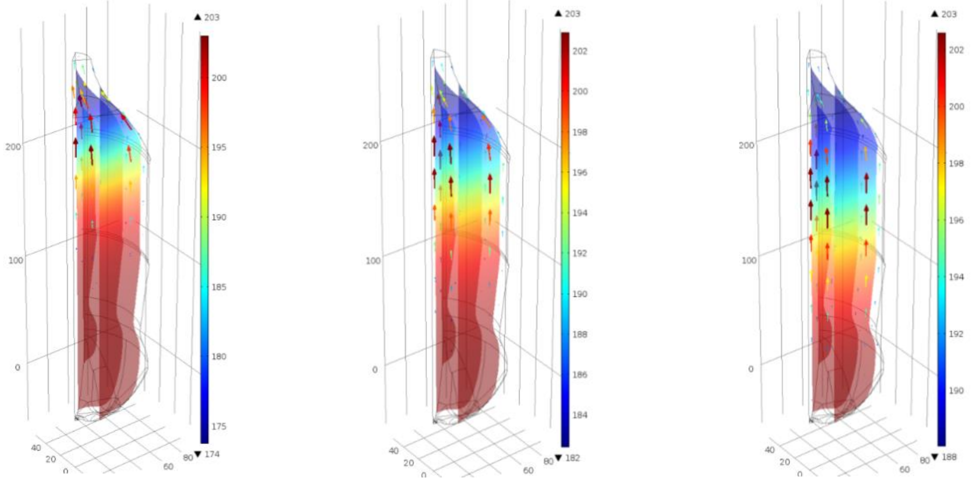
P_{CO_2}	$\mathrm{mod1.C_2} * \mathrm{V_1} * 10^{-6}\,[\mathrm{m^3/mol}]/(\frac{\mathrm{V_2}}{\mathrm{Rconst} * \mathrm{T}} + \mathrm{H} * \mathrm{V_1})$
H	0

2.3.6. Finite Element Analysis of Current Production Conditions

The finite element method was first used to look at how much gas was lost over time in a 2.5 L cola drink made under current conditions. Figures 10 and 11 show how the molar concentration changes over time, and Figure 12 shows the total gas loss curve over 180 days. This makes it clear from the start which way the CO2 is moving in the liquid. The gas in the fluid, which is the dense medium, moves quickly to the top, which is the less dense medium. This transport keeps going quickly until it reaches perfect balance. After that, the speed gradient slows down over time. This movement continues both toward the top and through the PET bottle wall to the external atmosphere until the molar concentration reaches zero. The main focus of the study is the slowing down of the gas loss rate over time, and the numerical effects of the variable parameters affecting this rate have been clearly demonstrated through the studies. Based on the data obtained, idealized production recipes were implemented in the field, and the results were validated with values obtained using the finite element method. This study can be used as a reference for all bottle types and production plants.

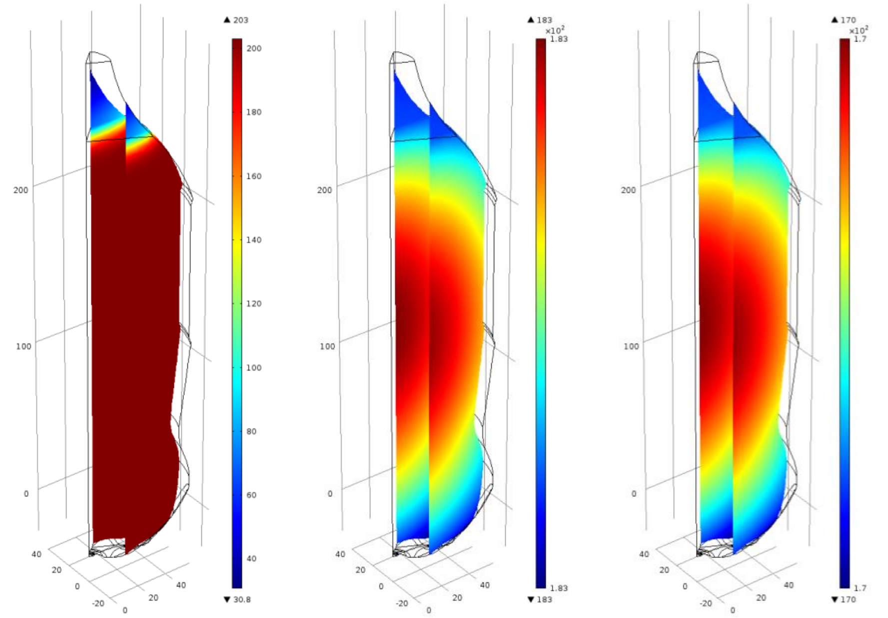


Time=0 s Time=60 s ZTime=600 s



Time=1800 s Time=3000 s Time=4800 s

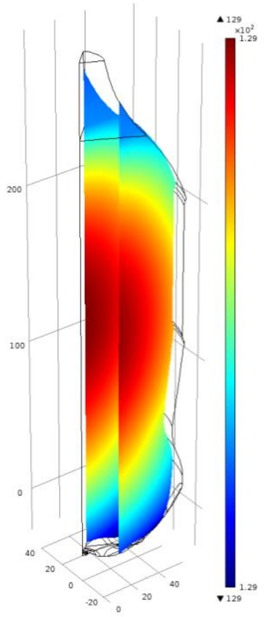
Figure 10. Direction of movement of CO_2 gas between 0-4800 s.



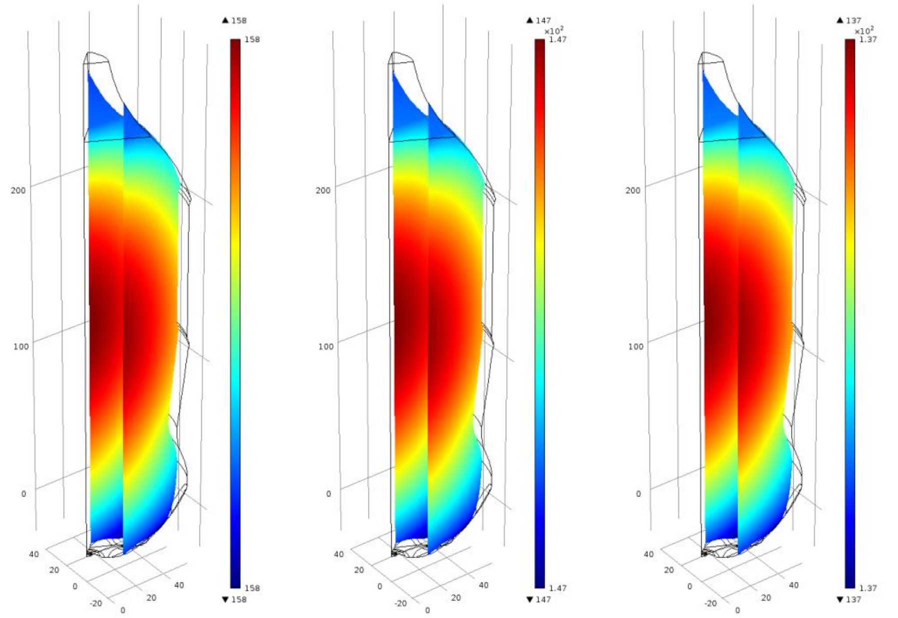
T=289 K, thickness=0.25 mm Time=0 day

T=289K thickness=0.25 mm, time=30th day

T=289K thickness=0.25 mm, time=60th day



T=289K thickness=0.25 mm, time=180th day



T=289K thickness=0.25 mm, time=90th day

T=289K thickness=0.25 mm, time=120th day

T=289K thickness=0.25 mm, time=150th day

Figure 11. Direction of movement of CO_2 gas for 0-180 days (T=289 K; t=0.25 mm).

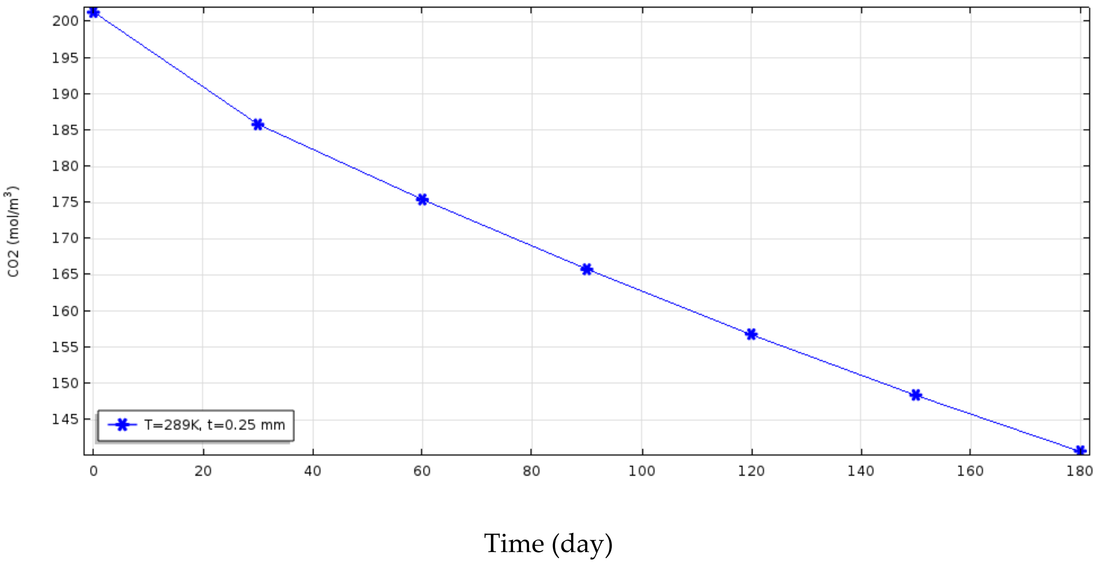


Figure 12. Time-dependent change of carbon dioxide gas between 0 and 180 days (T=289 K; t=0.25 mm).

As can be seen in Figure 12, the data obtained using the finite element method confirm the experimental study values and show that the gas amount decreased by 31% after 180 days. The agreement between the defined mathematical model and the experimental results has created a significant opportunity to monitor the effects of other variables. The effect of the other conditions defined as an improvement and development step of the study on gas loss will be demonstrated using a finite element numerical analysis program. The results obtained in this way will be used as a reference for experimental studies. Once these variables are implemented under real-world production conditions, the results are expected to be consistent with the values obtained from the finite element numerical analysis program. The effect of product storage temperature and the effect of the PET packaging wall thickness on total gas loss, as mentioned at the beginning of the study, will be demonstrated separately in the finite element numerical analysis program and will also be evaluated under real-world production conditions. As a result of all these analyses, the optimal conditions for a 2.5 L cola beverage will be determined.

2.4. Finite Element Numerical Analysis of the Effect of Storage Temperature

The consistent results obtained with the finite element analysis program for current production conditions made it possible to demonstrate the impact of other physical conditions on gas loss. By assuming temperature parameters as variables and other conditions as constant, the program enabled rapid analysis.

Figure 13 shows the effect of product storage temperature on the diffusion of dissolved CO_2 gas in cola beverages into the external atmosphere. When three different temperatures, 285 K, 289 K, and 291 K, were examined, it was revealed that gas loss decreased linearly with decreasing temperature and that there was a strong relationship with temperature.

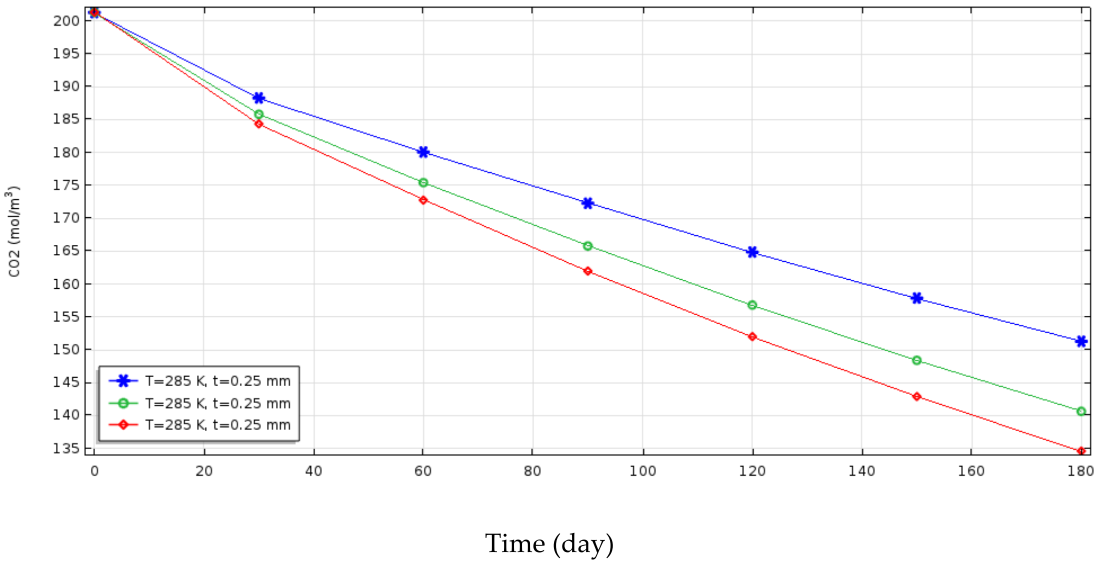


Figure 13. Change of CO_2 gas according to storage temperature for 0-180 days (T=285 K, 289 K, 291 K; t=0.25 mm).

Consequently, a cola product in a 2.5 L PET bottle stored at 285 K experienced 12% less gas loss after 180 days than a product stored at 291 K. The temperature variable is considered a significant factor and has been the subject of research in numerous articles in the past. While managing temperature input is challenging until the final product reaches the market, maintaining a storage temperature of 277 K-279 K for products stored in refrigerators in the market offers a significant advantage in ensuring high-quality products reach customers.

These findings provide an important guide for determining the optimal storage conditions for cola beverages. The study thoroughly investigated the impact of product storage temperature on total gas loss, as previously indicated, and demonstrated this under actual production conditions.

2.5. Finite Element Analysis of Regional Gas Loss in PET Bottles

After examining in detail the effect of temperature on the time-dependent change of dissolved CO_2 gas in cola beverages, the effect of PET bottle wall thickness, another variable in the doctoral dissertation, on gas loss was also analyzed.

It is a fact that increasing the wall thickness along the length of the PET bottle will positively impact gas loss due to its barrier properties. However, due to the increasingly challenging competitive environment, manufacturers' desire to minimize material use leads to the desire to use lighter-weight preforms. This can lead to significant financial gains and the opportunity to offer cheaper products in competitive markets.

The original study aimed to reduce gas loss by maintaining the existing preform weight constant and changing the material distribution in the PET bottle's partial regions. In this context, gas loss over time was analyzed based on the sub-sections, which are the main regions divided into sections (Figure 14). The target region for the study was defined according to regional differences, and the effect of the change in this region on reducing the time-dependent gas loss was measured under real production conditions, and the results of the finite element numerical analysis were verified.

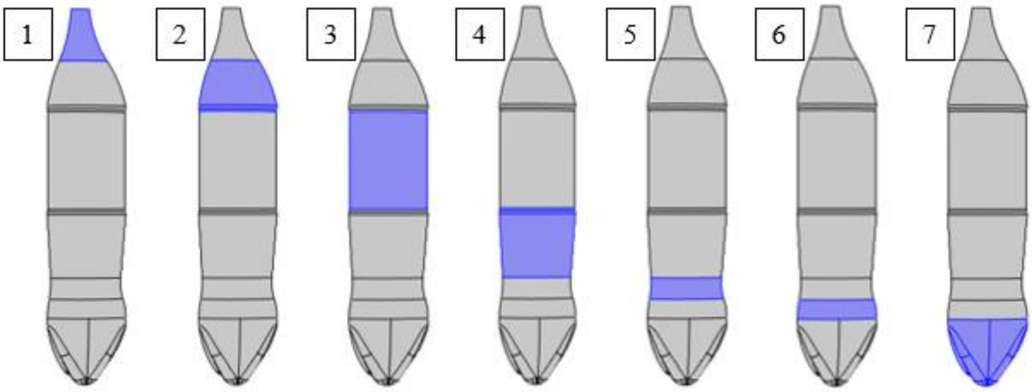
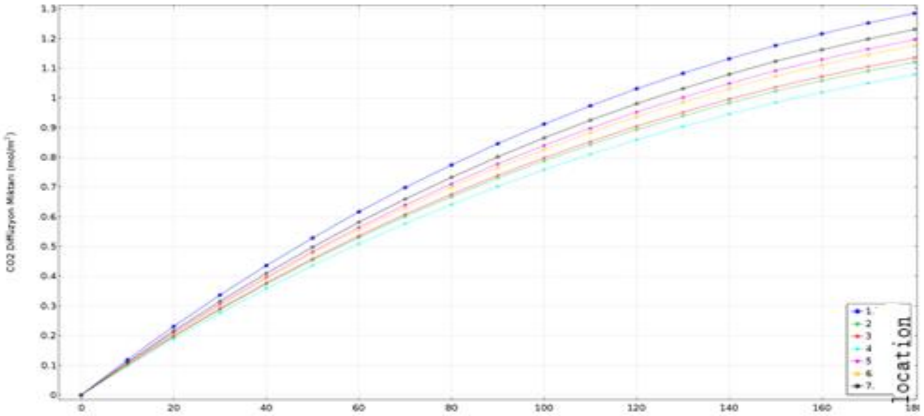


Figure 14. PET bottle physical region definitions.

As can be seen in Figure 15, the analysis revealed that the time-dependent gas loss from the shoulder region of the 2.5 L PET bottle is greater than in other regions. The primary objective will be to define this region as the target region and structure the material distribution to maximize this region. Using a finite element numerical analysis program, the thickness of this region will be defined as a variable, and the effect of varying the wall thickness of this region on the gas loss of a 2.5 L cola beverage over a 0-180 day period will be demonstrated. The wall thicknesses defined as variables in this region were also adapted to production conditions, and the results were compared.



Time (day)

Figure 15. Time-dependent change of CO_2 gas from PET bottle-defined regions for 0-180 days (T=289 K; t=0.25 mm).

2.6. The Effect of PET Bottle Shoulder Wall Thickness on Gas Loss

As can be seen in Figure 16, the greater time-dependent gas loss in the bottle shoulder region led to this area being selected as a target. Three different thickness values of 0.25 mm, 0.30 mm, and 0.35 mm were selected and analyzed, in line with the limits allowed by the production machinery without disrupting the physical structure of the existing PET bottle.

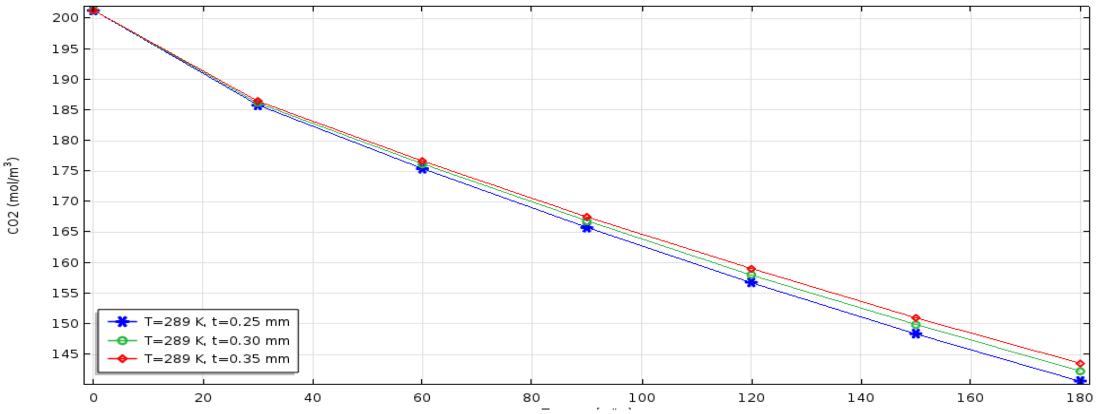
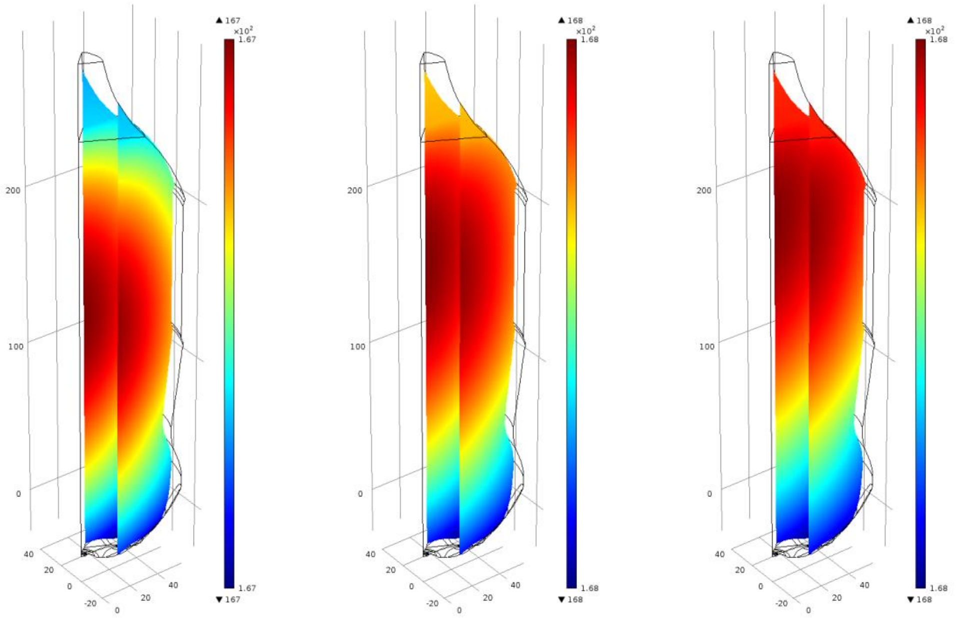


Figure 16. Effect of 0-180 day PET bottle shoulder part wall thickness on CO_2 gas change (T=289 K; t=0.25 mm, 0.30 mm, 0.35 mm).

Figure 16 shows that as the thickness of the bottle shoulder increases, the time-dependent change in dissolved carbon dioxide in cola beverages decreases. By further increasing the thickness within the limits allowed by current production machinery, we can significantly improve this situation.

2.7. Finite Element Analysis of the Combined Effect of Variable Temperature and PET Bottle Shoulder Wall Thickness on Gas Loss

To establish an experimental model of ideal production conditions and to observe the effect by applying it to real-world production conditions, the combined effect of optimal temperature and optimal bottle shoulder wall thickness on gas loss with time will be investigated using a finite element numerical analysis program. Thus, the crucial phase of the doctoral study, ideal production conditions, will be analyzed with a finite element analysis program, and the results will be observed by applying ideal boundary conditions to real-world production conditions. These results will be crucial for evaluating different boundary conditions. As a further validation of the function used, the mass production results will be an important indicator of the effectiveness of the function parameters. Figures 17 and 18 show the time-dependent effects of varying temperature and bottle shoulder wall thickness on total gas loss. Figure 19 shows the general trend for different values of these two parameters, demonstrating the situation more clearly.



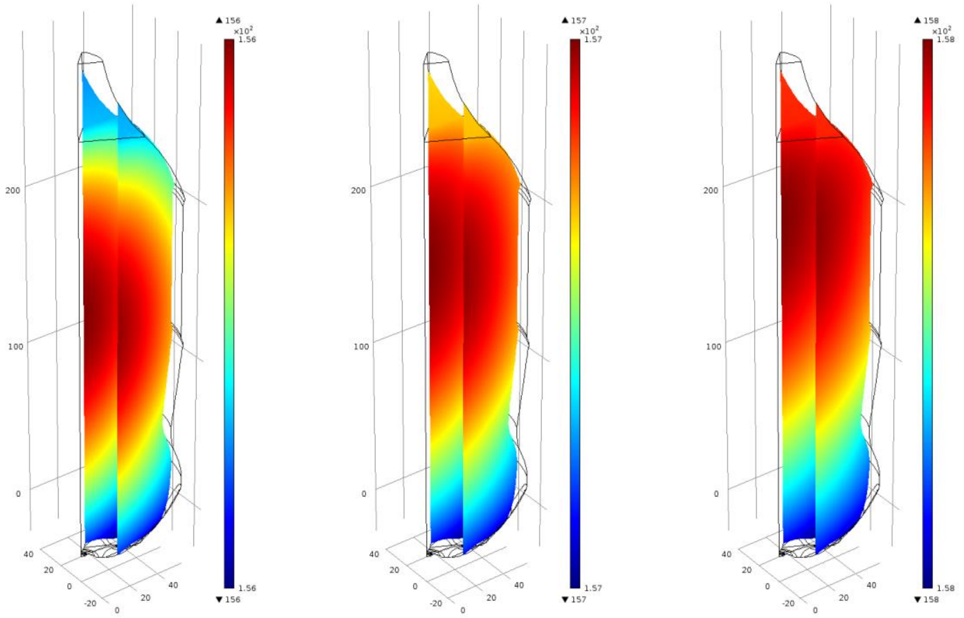
T=278K Thickness=0.25

mm

T=278K Thickness=0.30

mm

T=278 K, Thickness=0.35 mm



T=283K Thickness=0.25

mm

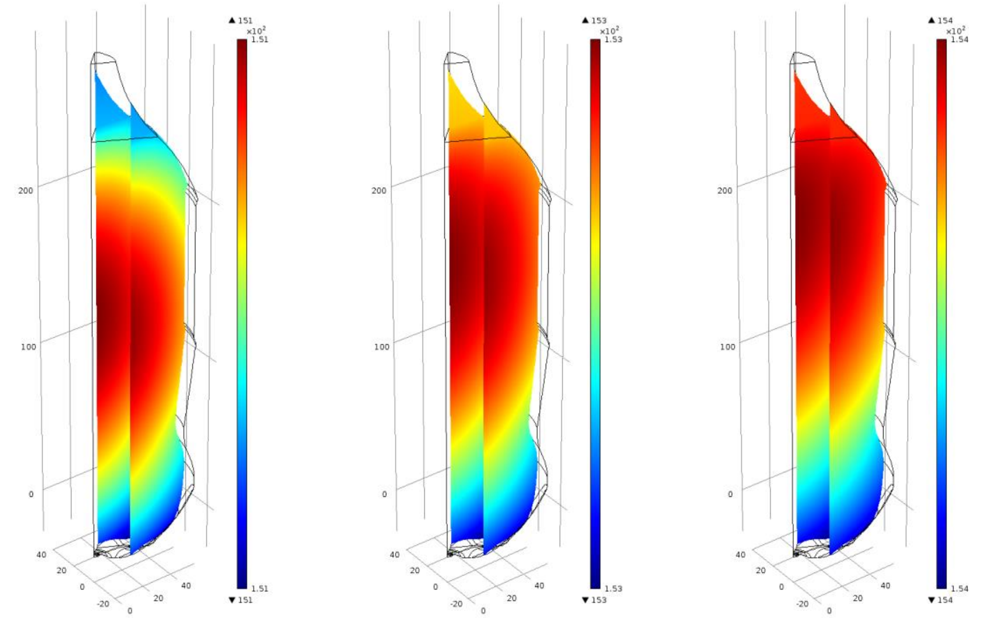
T=283K Thickness=0.30

mm

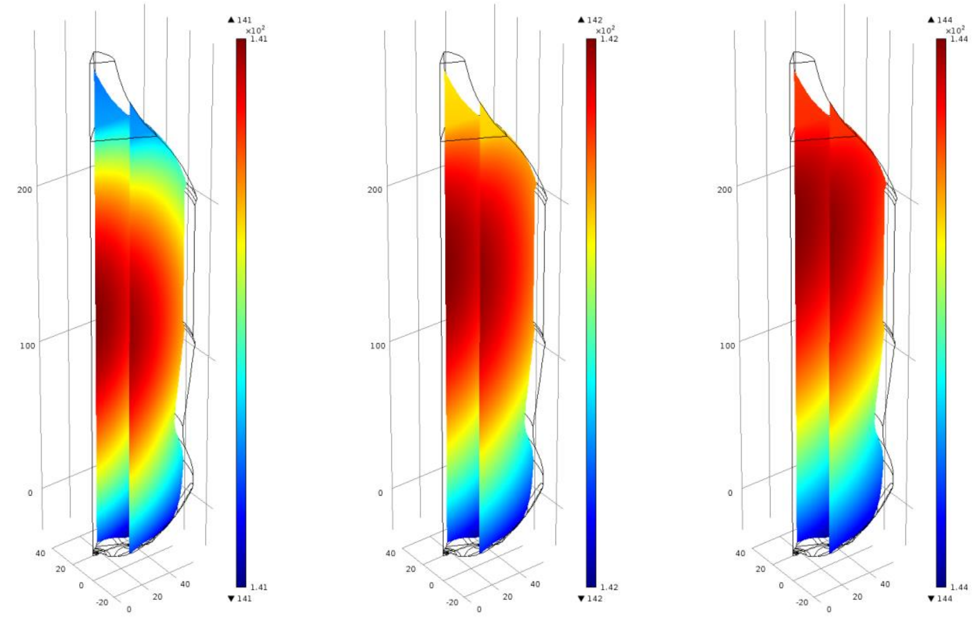
T=283K Thickness=0.35

mm

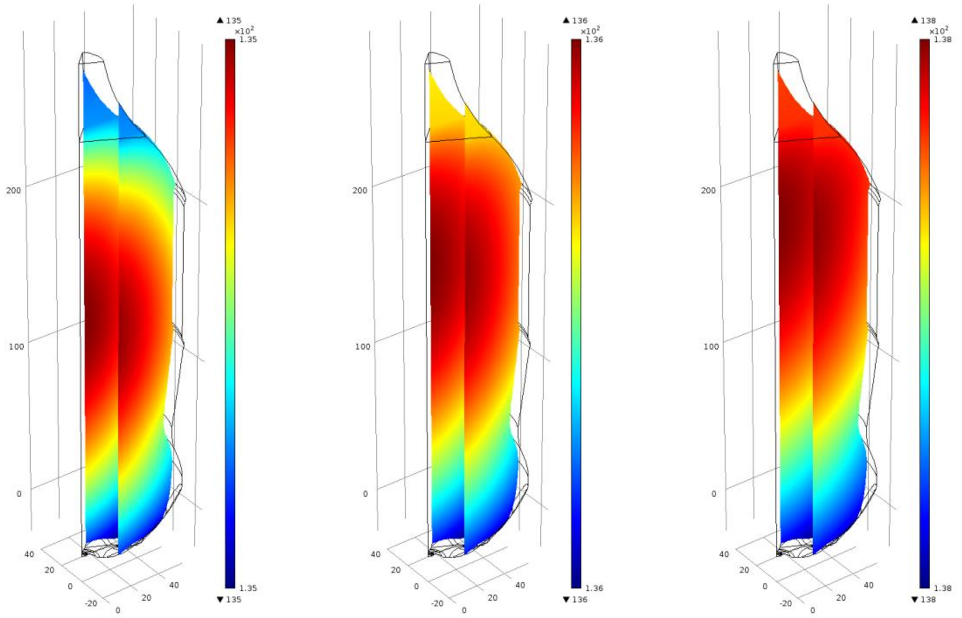
Figure 17. PET bottle shoulder region thickness after 180 days and the effect of product storage temperature change (T=278 K, 283 K; t=0.25 mm, 0.30 mm, 0.35 mm).



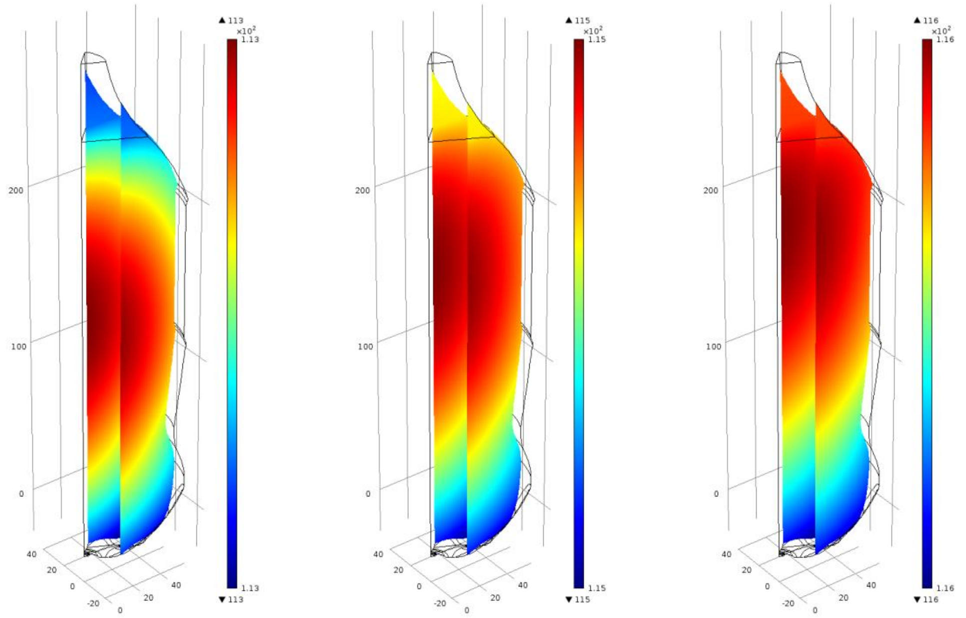
T=285 K, Thickness=0.25 mm T=285 K, Thickness=0.30 mm T=285 K Thickness=0.35 mm



T=289 K, Thickness=0.25 mm T=289 K, Thickness=0.30 mm T=289 K, Thickness=0.35 mm



T=291 K Thickness=0.25 mm T=291 K, Thickness=0.30 mm T=291 K, Thickness=0.35 mm



T=298 K, Thickness=0.25 mm T=298 K Thickness=0.30 mm T=298 K, Thickness=0.35 mm

Figure 18. Effect of CO_2 gas on PET bottle shoulder region thickness and product storage temperature change after 180 days (T=285 K, 289 K, 291 K, 298 K; t=0.25 mm, 0.30 mm, 0.35 mm).

doi:10.20944/preprints202603.2273.v1

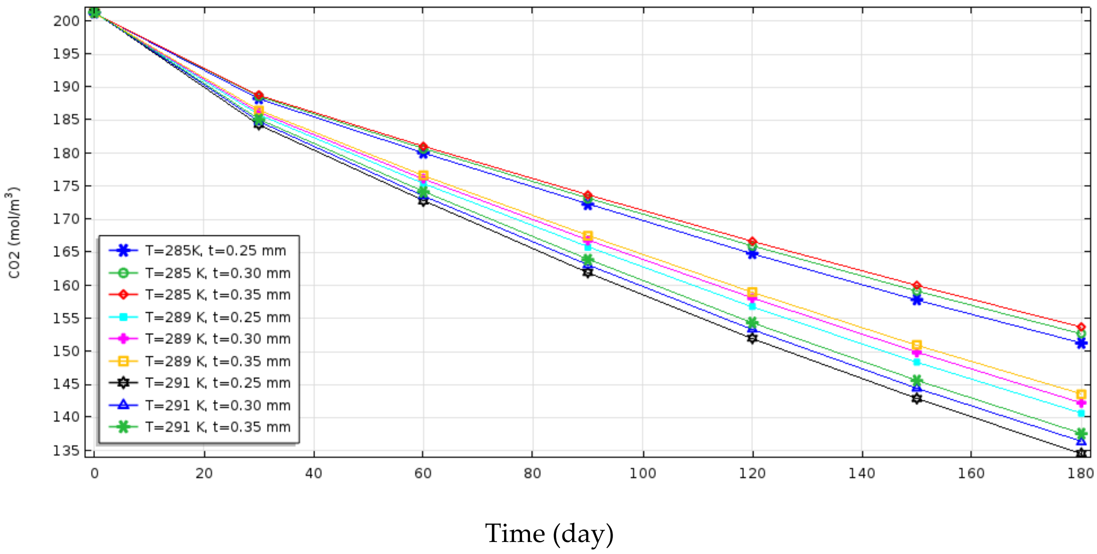


Figure 19. Effect of product storage temperature and PET bottle shoulder region wall thickness changes on the amount of CO_2 gas diffusion after 180 days.

As can be seen in Figure 19, as the product storage temperature decreases and the bottle shoulder thickness increases, the diffusion of CO_2 gas decreases over time. In this case, the analysis results indicate that a product temperature of 285 K and a bottle shoulder thickness of 0.35 mm constitute ideal production conditions.

Figure 20 shows the time-dependent diffusion trend of dissolved carbon dioxide gas in a 2.5 L cola beverage, which depends on the ideal production temperature and bottle shoulder area thickness.

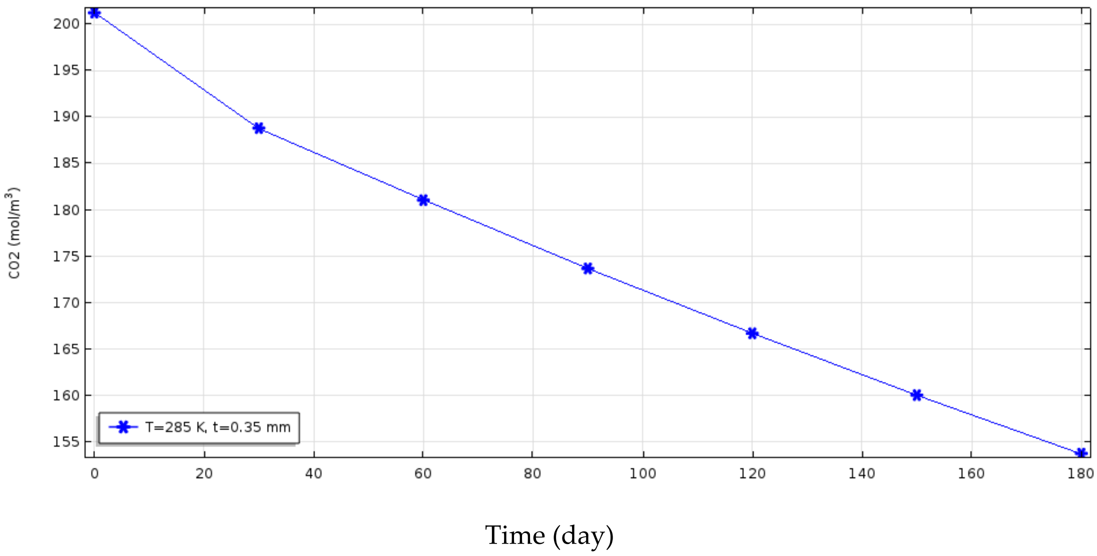


Figure 20. Change in the diffusion of CO_2 gas with time (T = 285 K; t = 0.35 mm).

3. Adaptation and Analysis of Variables to Production Conditions

3.1. The Effect of PET Bottle Shoulder Wall Thickness on Time-Dependent CO_2 Gas Diffusion

PET bottles can have different technical dimensions depending on their design and the technology used. The manufacturer's design specifications determine the preform type and weight. As companies increasingly fill bottles with lighter weights in growing competition, this translates to significant economic gains depending on production volume. On the other hand, this situation, especially for sparkling beverages, brings with it disadvantages in terms of quality. Depending on the wall thickness of PET bottles used, the CO_2 gas contained within decreases over time. One of the important outcomes of this doctoral thesis is the ability to offer high-quality products using low preform weight without increasing costs in a competitive market. The economic benefit of this study is quite significant for sparkling beverage manufacturers with large production volumes.

This part of the study involved defining the material distribution on the bottle as a variable using finite element software and interpreting the molar change of CO_2 gas dissolved in the cola inside the PET bottle for each variable value. Based on the results obtained from the finite element numerical analysis program, the variables were applied to actual production conditions, and bottles meeting quality standards were produced. The bottles were filled, keeping the production temperature and storage conditions constant, and then they were stored in an idealized environment under constant temperature conditions for periodic measurements. Based on the improvements obtained, the PET bottle production process was made suitable for mass production. The production process, which achieved ideal material distribution, was checked for suitability for mass production, and gas loss measurements were periodically made on bottles produced under these conditions. To ensure the same quality bottles under mass production conditions:

- Infrared lamps were modified, and heating power was increased.
- Heating lamps were lowered toward the preform ring region.
- Pressurization times were adjusted, and the P_1 pressure range was increased to 15-16 bar.

According to the results obtained from the finite element numerical analysis, bottles with the same material distribution as the current production conditions could be produced, and production recipes covering all settings on the machines were created to ensure that these production values remain stable. Continuous measurements were taken to verify bottle quality and keep variables under control. A key priority was ensuring that these mechanical and process revisions were simple to implement and did not impact other bottle types. In other formats of production, such as 1L or 2L, it is of extreme importance for quality that these changes can be converted to format-specific values. The machine's technology allows for easy adjustments to the desired values, and production can be done at the same standard values.

Figure 21 shows the measurement results from PET bottles produced with changes made to actual production conditions. The 2.5 L cola beverage, produced with the temperature variable kept constant, was kept in environments where storage conditions could be kept under control, and the results were measured periodically. Samples taken from the production line were immediately measured and recorded as the initial reference value for each sample.

Effect of wall thickness on total CO_2 diffusion (Month 6)

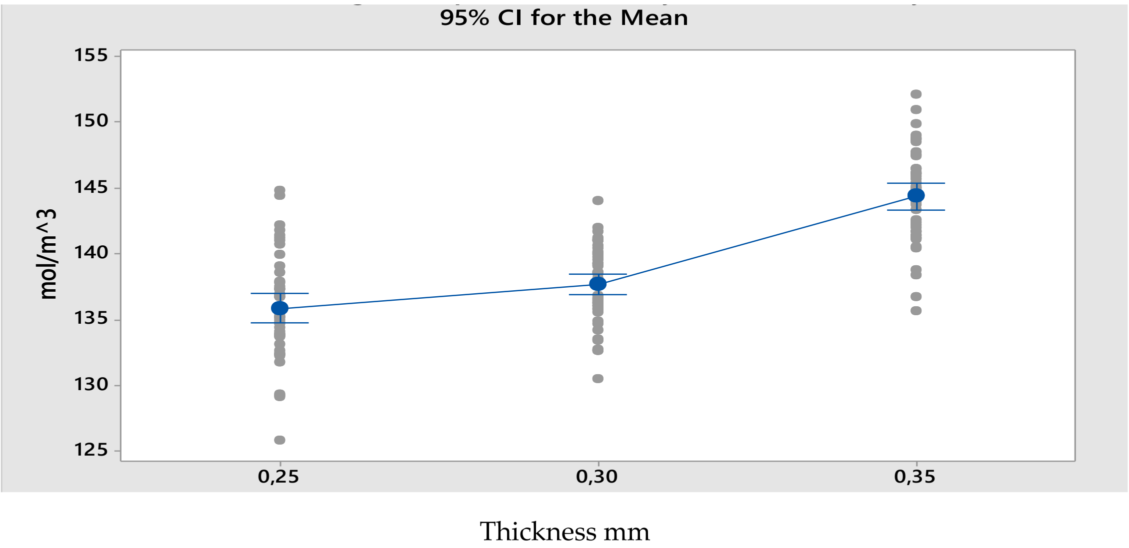


Figure 21. Effect of PET bottle shoulder region wall thickness on the time-dependent change of CO_2 gas (T = 289 K; t = 0.25 mm, 0.30 mm, 0.35 mm).

As can be seen in Figure 21, it is clearly demonstrated that gas loss is higher in the reference bottle produced with a wall thickness of 0.25 mm (14.5 g) compared to the 0.30 mm (17 g) and 0.35 mm (19 g) wall thicknesses. Experimental data indicate that the 2.5 L PET bottle produced with a wall thickness of 0.35 mm provides a 4.5% better barrier property. The results of the experimental studies and the values obtained using the finite element method are consistent, indicating that increasing the wall thickness of the PET bottle shoulder region is an important variable for reducing total gas loss.

3.2. The Effect of Storage and Production Temperature on Time-Dependent CO_2 Diffusion

Finite element numerical analysis has demonstrated that product filling temperature and storage conditions are significant variables in the time-dependent change of dissolved CO_2 gas in cola products. While the filling temperature of cola beverages can be adjusted as desired using precise control equipment, storage conditions can vary until the product enters the refrigerator at the store. In this section of the study, the filling temperature and storage temperature of cola beverages produced at different temperatures were adjusted to create an environment where they remained constant, and the change in gas loss over time was examined. As is known, temperature input is the primary function of the diffusion concentration gradient in gases. The gas contained in bottled cola beverages, which have a high density, will diffuse rapidly into the lower-density external atmosphere. Temperature has a direct impact on this diffusion rate. Gas molecules will move faster with changing temperature. Samples taken from the production line were considered as the initial reference value, and the total change was determined based on this reference value.

Effect of temperature on total CO_2 diffusion (Month 6)

As can be seen in Figure 22, the gas loss of 2.5 L cola beverages produced at 12 ℃ (285 K), 16 ℃ (289 K), and 18 ℃ (291 K) was examined under storage conditions at the same temperatures, and the effect of temperature on total gas loss was shown. The measurement results indicate that cola beverages produced and stored at 285 K contained 13.2% more dissolved carbon dioxide than cola beverages produced at 291 K. This situation limits the temperature factor, which is considered a significant variable and forms a crucial cornerstone of the quality journey from production to the customer. Although the temperature input can be kept within certain ranges at the production site, managing this variable during the journey to the market is not simple for every company. Consequently, the analyses and results in this study were modeled based on conditions within the production facility, and the process leading to the market was neglected. This was very important in keeping products from being lost because there wasn't enough stock or there were problems with production during the busy summer months. One of the main goals of carbonated beverage companies is to give customers high-quality products. This is the main idea of this doctoral dissertation. Consequently, the temperature input of carbonated beverages will be analyzed in the resultant numerical model, and the variation in gas content of cola beverages in PET containers subjected to different temperatures for designated durations will be thoroughly investigated in the subsequent study.

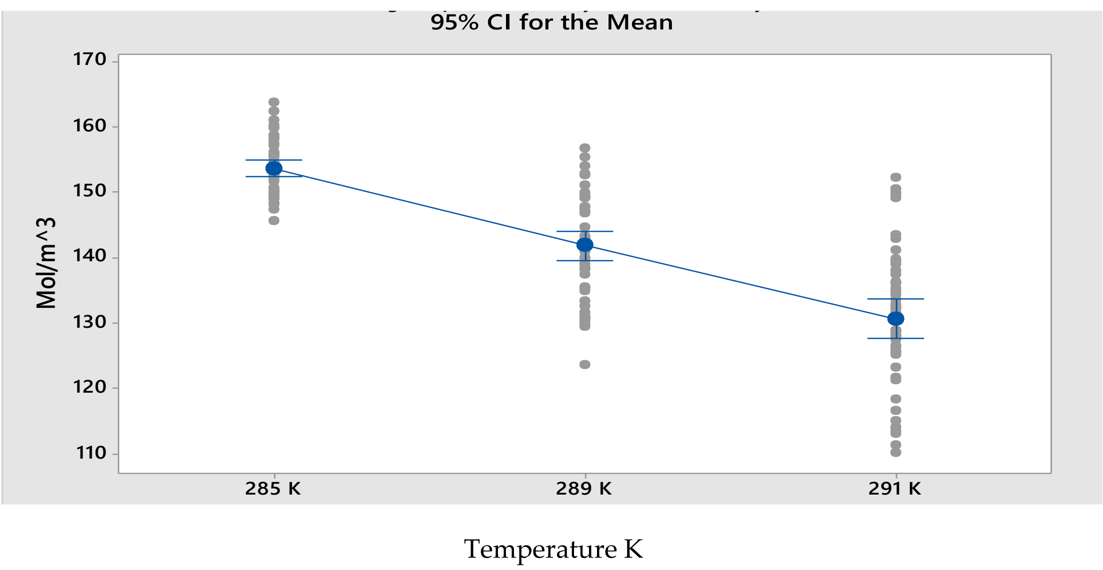


Figure 22. Effect of filling and storage temperature on the time-dependent change of CO_2 gas (t = 0.25 mm).

It is an inevitable fact that production temperatures as well as storage conditions must be managed in the best possible way. The temperature-dependent retention of dissolved CO_2 gas in the fluid and its solubility are significantly influenced by temperature. The temperature limits of the filling process vary depending on the adequacy of the technology used. This comes with a number of important control parameters. When production happens at high temperatures, the dissolved CO_2 gas moves quickly to the top, which causes foaming problems. This means that a lot of bottles that don't keep their product levels stable are thrown away. Also, making things at low temperatures can cause valves to get stuck and big production losses, depending on how fast the production is and what technology is used, as well as the type of crystal sugar used. As a result, manufacturers have had to run many tests to find the best temperature. In this study, the state-of-the-art technology has enabled production at a wide range of temperatures, enabling rapid production.

3.3. The Effect of Ideal Production Temperature and PET Bottle Material Distribution on Time-Dependent CO_2 Gas Diffusion

Based on the values obtained from experimental results, ideal production conditions were defined, and production was carried out under these conditions. The filling temperature of the 2.5 L cola drink produced under mass production conditions was ensured to be 12 °C and the PET bottle shoulder area thickness was 0.35 mm, and the necessary measurements were made from samples taken at certain intervals and the standard deviation was verified as 0.1 mm for both temperature and material thickness. The produced bottles were first subjected to quality tests to confirm compliance with production conditions and to verify that there were no obstacles to their sale. After initial measurements, each 2.5 L cola beverage was labeled and placed in a controlled storage area. The amount of gas contained over time was measured at the frequency determined by the quality department staff and recorded for each.

Figure 23 shows the time-dependent effect of idealized temperature and material distribution on gas loss. It was noted that the total gas loss of bottles made under perfect production conditions went down by 37% over six months. We made a change curve by recording the average change of 50 bottles at the specified frequency. The change graph shows that the rate of change went down by this amount, which shows that the curve from the study's finite element analysis is similar.

Pre

Post
5,1 bar-t 0,25 mm T= Depo
5,1 bar- t 0,35 mm T= 12°C
Pre-Post Analysis
1st M 2nd M 3rd M 4th M 5th M 6th M

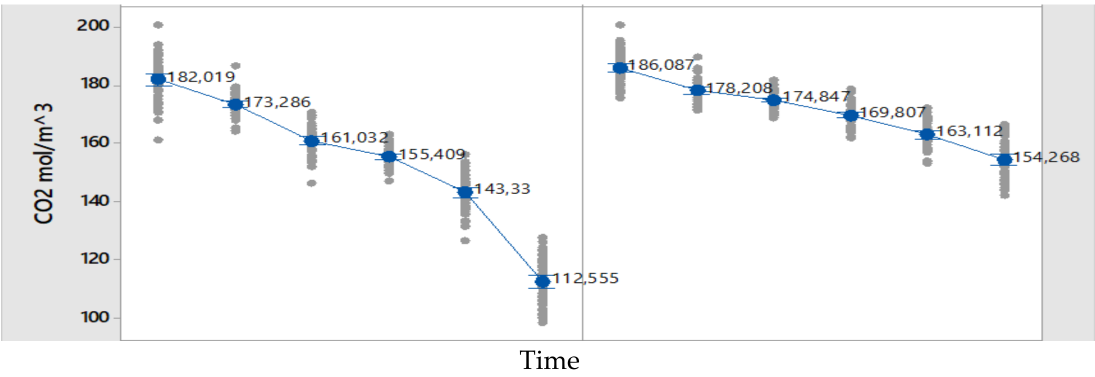


Figure 23. Change in CO_2 gas over time in a 2.5 L PET bottle packaged cola drink produced under ideal production conditions.

4. Conclusion

This study looked into the main reasons why the amount of CO_2 gas in cola drinks in PET bottles goes down over time. This is an important part of the carbonated beverage industry. Improvements have given us a new way to look at the production process. PET packaging offers significant advantages over other packaging types in terms of ease of production and cost, making it an indispensable material for the beverage industry. Investing in PET production is one of the best ways to make money in the growing beverage market. So, the results of our study are very important for all companies that make carbonated drinks that come in PET packaging. This study looks at how the barrier properties of PET packaging affect gas loss, which is what many other studies have looked at in the past. Earlier research has solely investigated the thermophysical characteristics of PET. This study, however, suggests enhancement techniques associated with the optimization of variable parameters. This distinctive feature of the study can act as a reference for both manufacturers of machines and production facilities. This study investigates the interplay between temperature and the thermophysical properties of PET materials, showcasing experimental modeling outcomes that integrate both variables, thereby facilitating the generation of data that closely approximates the precision attained in actual production environments. Even though the experiments and analyses were done on a 2.5-liter package, the study's unique structure showed that it was valid for all other package sizes and that it could be used by everyone in the industry. Consequently, the sector examined in this study encompasses not only cola producers but also possesses considerable significance for all industries utilizing CO_2 gas. This study is unique because it uses real-world simulation analysis with the finite element method to find target points, which is different from other literature studies. Another important part of this study is the separate evaluation of temperature conditions and optimized PET material distribution using both experimental and finite element analysis. The finite element method results were compared to the experimental results, and the results of different variables within the parametric diffusion function were also looked at. So, the results were looked at all together, and the best temperature for making PET bottles was found.

As a result, it was determined that reducing the product filling temperature and increasing the pressure reduced the diffusion of dissolved carbon dioxide gas from the packaging to the external atmosphere. It was also noted that making the shoulder area of the bottle thicker slowed down the loss of carbon dioxide gas over time. Based on the results, standardized production recipes led to consistent performance, and the following results, which can be used as a model for other types of packaging, were achieved:

At the end of the sixth month, the molar diffusion rate in 0.35 mm-thick PET bottles was 5.2% less than that in 0.25 mm-thick PET bottles when comparing the two types of bottles.

- At the end of the sixth month, the time-dependent molar gas exchange of the cola beverage at a production temperature of 285 K decreased by 13.2% compared to a production temperature of 291 K.

- The sudden loss rate after the first and fifth months of production decreased by 30% due to the improvement.
- A 37% improvement has been achieved under ideal production and storage conditions compared to current production conditions. The longer shelf life resulting from this improvement is considered an economic gain, and it has also been a significant step forward in meeting the high demand during the summer months. This improvement, achieved within a sustainable quality approach, has also had a significant impact on the more effective use of resources.

Considering the features listed above, gas losses occurring after the first and fifth months will be largely controlled, enabling more planned and higher-standard production for the sparkling beverage industry. Furthermore, consumer complaints will be minimized, bringing significant benefits such as reducing investment and production costs.

The holistic findings of the study indicate that the shelf life of cola beverages can be significantly extended if PET bottles are produced to the optimum thickness and temperature control is ensured during storage/logistics processes. In this context, the following recommendations are made for manufacturers:

- Material distribution in PET bottles should be optimized, especially in the shoulder area.
- Low temperatures should be preferred during filling operations.
- The cold chain should be maintained during storage and logistics processes.
- Future studies should also investigate temperature fluctuations and different preform material combinations under real-world conditions.

In conclusion, this study highlights the criticality of evaluating temperature and wall thickness in PET-packaged cola beverages for shelf life optimization, offering both scientific and practical contributions to the food industry.

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