



UNIVERSITY OF CONNECTICUT

**OPIM 5770-Advanced Business Analytics and Project
Management**

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1. Executive Summary

This project focuses on optimizing the production process for PET bottles at PepsiCo, specifically targeting inefficiencies in the Stretch Blow Molding (SBM) process. These inefficiencies, primarily driven by suboptimal material distribution, lead to excessive plastic usage, increasing production costs and conflicting with PepsiCo's sustainability goals for 2025. A predictive model was developed to assess and optimize bottle performance based on manufacturing parameters such as section thickness, aiming to reduce material usage while maintaining strength and integrity.

A dataset of four preform types with varying weights, shapes, and materials was used, including critical SBM parameters, section weights and thicknesses, and performance metrics (Thermal Stability, Empty Top Load, and Burst Tests). Through exploratory data analysis (EDA) and predictive modeling, key factors influencing bottle performance were identified, and models were created to predict performance based on section characteristics.

The predictive models showed strong performance for metrics like Burst Expansion and Empty Top Load, with R^2 values exceeding 0.95 for many preforms. However, Thermal Stability showed mixed results, indicating that some metrics are better suited for machine learning (ML) predictions, while others require traditional testing for validation. Optimizing material distribution, particularly in the shoulder, grip, and base sections, can significantly reduce plastic usage without compromising bottle integrity.

Here are some final recommendations:

- Focus on optimizing Sth2–Sth5 thickness to enhance thermal performance across all bottle types.
- Maintain balanced thickness distribution in the grip and shoulder sections to improve Empty Top Load resistance.
- Use ML models for metrics like burst testing and top load performance for AXL bottles, while retaining traditional testing for Ripple bottle top load and AXL thermal expansion.
- Optimize the 20.5g AXL bottle to reduce plastic usage while maintaining performance, aligning with sustainability objectives.

2. Problem Statement

PepsiCo's blow molding process for PET bottles currently encounters inefficiencies primarily driven by suboptimal material distribution resulted by Stretch Blow Molding (SBM) recipes. These inefficiencies lead to excessive plastic usage, which not only elevates production costs but also conflicts with PepsiCo's sustainability goals for 2025. As the company aims to minimize environmental impact, the overuse of plastic in bottle manufacturing presents a critical challenge. This project seeks to address these inefficiencies by developing a predictive model to assess and optimize bottle performance based on key manufacturing parameters, particularly section thickness. By accurately predicting performance, this model can guide adjustments to SBM recipes, allowing for reductions in material usage while maintaining essential strength and integrity requirements. The ultimate goal is to advance toward a more resource-efficient production process, in alignment with PepsiCo's sustainability commitments.

3. Methodology

To address the challenge of optimizing material distribution in PET bottles, a structured approach was followed to develop a predictive model that aligns with both performance and sustainability goals. Initially, comprehensive data preparation and cleaning ensured the quality and reliability of the dataset, followed by an Exploratory Data Analysis (EDA) examining univariate, bivariate, and multivariate relationships. This analysis provided insights into the influence of manufacturing parameters on bottle performance, particularly the relationship between section thickness and strength metrics. In building the predictive model, the data was split into training and testing sets, with a focus on enhancing model interpretability and accuracy through feature engineering, hyperparameter tuning, and interaction terms. The model's performance was evaluated using the R^2 metric, guiding recommendations for recipe adjustments in the Stretch Blow Molding (SBM) process to achieve efficient material usage without compromising bottle integrity.

3.1 Data Description

The data includes key parameters relevant to PepsiCo's blow molding process for PET bottles. These parameters are measured across different sections of the bottle to assess performance and material distribution.

3.1.1 Overview of Data sets

Our dataset includes information on three distinct PET bottle preforms, each with unique properties that impact bottle performance:

- **Preform 1:** A 21.5g AXL bottle made from Bariq PET material. This preform has a distinct weight that influences material distribution, allowing us to study the effects of additional plastic on bottle strength and stability.
- **Preform 2:** A 20.5g AXL bottle made from DAK Perpetual PET material. Sharing the same shape as Preform 1 but with a lighter weight, preform 2 offers insights into how material reduction affects performance in an otherwise similar design.
- **Preform 3:** A 20.5g Ripples bottle, also made from DAK Perpetual PET. With a different shape than the AXL bottles, this preform introduces further variability in thickness distribution and performance metrics, highlighting the impact of design variations.
- **Preform 4:** A Ripple bottle with the same shape as Preform 3 but made from FENC PET material. This preform enables a comparative analysis of material properties between FENC and DAK Perpetual PET, focusing on their influence on thermal expansion and structural integrity.

Each preform is molded using a specific set of Stretch Blow Molding (SBM) parameters which directly influence the thickness distribution across bottle sections. This variety in weight, shape, and material type across the preforms allows for a comprehensive analysis of how these factors, combined with manufacturing parameters, affect overall bottle performance.

3.1.2 SBM recipe Inputs

The SBM recipe inputs include critical parameters such as Neck Temperature, Mass Flow Rate, and Preblow Timing, which play a fundamental role in shaping each bottle. These inputs are pivotal in determining the material properties and the thickness distribution across the bottle's sections, ultimately impacting the bottle's strength, flexibility, and overall performance.

3.1.3 Section Weights and Thickness

The weights and thicknesses of the bottle provide insights into how the SBM recipe affects the physical characteristics of the bottle across its structure.

3.1.3.1 Section Thickness

This includes thickness measurements across 15 levels of the bottle, divided into distinct sections.

- Top Section: Thickness at levels sth1 and sth2.
- Upper Panel Section: Thickness at levels sth3 to sth7.
- Lower Panel Section: Thickness at levels sth8 to sth13.
- Base Section: Thickness at levels sth14 and sth15.

3.1.3.2 Section Weights

This includes corresponding weights for each section (shoulder, label, grip, and base), with a constraint that the total weight of all sections sums to a constant.

3.1.4 Performance Metrics

The dataset includes three critical performance metrics that ensure the structural integrity and stability of carbonated PET bottles throughout their lifecycle. Each test is designed to address specific conditions that bottles may encounter during production, storage, distribution, and consumer use.

3.1.4.1 Thermal Stability

- Purpose: Ensures that PET bottles maintain dimensional stability and do not experience excessive deformation (creep) under real-world conditions. Dimensional changes in pressurized bottles may cause the liquid fill level to drop, impacting appearance and fit.
- Test Method: Bottles are placed in an environmental chamber with controlled temperature and humidity. They are marked and measured at specific locations (upper bumper, upper panel, middle panel, lower panel, lower bumper, and base). After testing, the percentage expansion at each location is recorded, with a passing criterion of no more than 3% expansion at any location.

3.1.4.2 Empty Top Load

- Purpose: This test measures the top load compression force of empty bottles to confirm that they can withstand the pressures applied by lift cylinders during filling and capping.
- Test Method: An Instron compression tester with a 0–100 kg load cell is used to apply force to the bottle until it reaches 3.75 mm deflection. The required minimum top load force for CSD bottles is 9.1 kg to ensure structural resilience.

3.1.4.3 Burst Test

- **Purpose:** Evaluates the bottle's resistance to internal pressurization, crucial for bottles containing carbonated beverages. The test ensures that bottles can withstand the rapid pressurization experienced during filling without failure.
- **Test Method:** Bottles are pressurized to 9.31 bar (135 psi) and held for 13 seconds, then burst pressure and expansion are recorded. For commercial CSD bottles, the target expansion during the hold phase is below 15%.

Each performance metric reflects the bottle's ability to meet industry standards, ensuring durability and minimizing material use without compromising quality.

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3.2 Exploratory Data Analysis

Exploratory Data Analysis (EDA) was conducted to uncover patterns, identify anomalies, and gain insights into the relationships among the different variables in our dataset. The primary focus was on understanding how various SBM (Stretch Blow Molding) parameters and preform characteristics affect bottle performance metrics.

3.2.1 Data Cleaning

The dataset utilized in this project was derived from controlled experimental conditions, ensuring that the data was well-structured and clean. Minimal issues were encountered concerning missing values, outliers, or inconsistencies. As a result, very few data cleaning steps were necessary, allowing for a concentration on analysis and modeling. The integrity of the data facilitated a smooth transition to the exploratory data analysis and predictive modeling phases.

3.2.2 Univariate, Bivariate, and Multivariate Analysis

3.2.2.1 Univariate Analysis

- **Techniques Used:** Box plots were created for each SBM recipe parameter, treated as categorical variables.
- **Rationale:** By visualizing the distribution of section thickness for each value of the SBM recipe parameters, insights were gained into how thickness varied with different recipe conditions. This analysis helped identify whether thickness increased or decreased in response to changes in parameters such as Neck Temperature or Mass Flow Rate.

3.2.2.2 Bivariate Analysis

- **Techniques Used:** Pair plots were employed to visualize relationships between section weights and thicknesses.
- **Rationale:** The pair plots demonstrated how changes in the thickness of one section affected the weights of other sections, highlighting the trade-offs necessary to maintain the fixed weight constraint across preforms.

3.2.2.3 Multivariate Analysis

- **Techniques Used:** Heatmaps were employed to explore the relationships between section thicknesses and performance metrics.
- **Rationale:** The heatmap revealed correlations between thickness measurements at different sections and performance metrics such as Burst Pressure and Thermal Expansion. Notably, thermal expansion was significantly influenced by thickness at specific locations.

3.2.3 Performance Metric Analysis

3.2.3.1 Thermal Expansion Analysis

Thermal expansion describes a material's response to temperature changes, where dimensions alter due to molecular vibrations. For PET (Polyethylene Terephthalate), a solid material commonly used for bottle manufacturing, expansion is primarily linear. The governing equation for linear thermal expansion is:

$$\Delta L = \alpha \times L_0 \times \Delta T$$

Where:

ΔL is the change in length.

α is the coefficient of linear thermal expansion

L_0 represents the initial dimension (in this case, thickness).

ΔT is the temperature change

Thicker bottle walls have greater initial dimensions, leading to more significant absolute expansion for the same temperature increase. This explains why bottles with higher thickness in sections sth1 to sth3 experience more expansion, making them prone to failure.

Additionally, thicker walls delay heat penetration, causing non-uniform expansion across the wall thickness. This difference in expansion rates between inner and outer layers creates internal stress, which can weaken the structural integrity of the bottle.

The observed failures can be attributed to increased thickness in sections sth1 through sth3. Excessive thickness leads to higher absolute expansion when exposed to heat, particularly impacting the upper panel. Moreover, the label section (sth3 to sth7) is critical for maintaining material consistency, and deviations in this area (such as a sharp thickness reduction) exacerbate the risk of non-uniform expansion, leading to structural failure.

3.2.3.2 Burst Expansion Analysis

The ability of bottles designed for carbonated or pressurized beverages to withstand rapid internal pressurization without failure is critical, particularly during the filling operation. Bottles that fail to handle this pressure can lead to significant production issues and pose safety hazards. To analyze the burst performance of the bottles, Laplace's Law was utilized, which describes the relationship between internal pressure, wall thickness, and the radius of the bottle.

For thin-walled pressure vessels like bottles, Laplace's Law can be expressed as:

$$\sigma_h = p r / t$$

Where,

σ_h = hoop stress (MPa, psi)

p = internal pressure in the tube or cylinder (MPa, psi)

r = internal radius of tube or cylinder (mm, in)

t = tube or cylinder wall thickness (mm, in)

This equation indicates that the hoop stress experienced by the bottle wall is directly proportional to the internal pressure and diameter, and inversely proportional to the wall thickness. As the wall thickness increases, the stress on the material decreases, leading to reduced burst expansion.

Burst expansion is inversely proportional to burst pressure, meaning that thicker walls require higher pressures to achieve the same level of expansion. Thus, thicker walls provide better resistance against burst failure by minimizing the expansion for a given internal pressure.

The correlation between the radius, wall thickness, and burst pressure provides valuable insights into design considerations for improving the robustness of PET bottles, ensuring they can withstand the demands of carbonated beverage packaging.

3.2.3.3 Empty Top Load Analysis

For the Empty Top Load performance metric, Euler's Buckling Formula was referenced to understand the bottle's behavior under vertical load. Euler's formula is given by:

$$P_{cr} = \frac{\pi^2 EI}{(KL)^2}$$

Where:

P_{cr} = critical load (N)

E = modulus of elasticity (N/m²)

I = moment of inertia (m⁴)

K = effective length factor (dimensionless)

L = unsupported length (m)

This formula indicates that the weakest sections of the bottle, characterized by lower diameter and reduced thickness are most susceptible to buckling under pressure.

Using this theoretical foundation, failed test cases were analyzed by focusing on the thicknesses at sections with lower diameters. This analysis enabled the identification of critical thickness ranges that are more prone to failure and differentiated them from those that successfully resisted top load pressures. By correlating these findings with overall bottle performance, a clearer understanding was gained of which thickness ranges are optimal and which should be avoided to prevent failure.

3.3 Predictive Modelling

In this section, the methodology adopted for developing predictive models aimed at optimizing bottle performance in the blow molding process is detailed. The goal is to build models that accurately predict key performance metrics while ensuring interpretability and generalizability across different bottle designs.

3.3.1 Data Preparation

3.3.1.1 Data splitting

The dataset was divided into training and testing sets using an 80-20 ratio. This split allows for training the models on a substantial amount of data while retaining a separate set for unbiased performance evaluation. The training set is used to fit the models, while the test set assesses how well these models generalize to unseen data.

3.3.2 Evaluation Metric

The primary metric for evaluating the models is the R^2 (coefficient of determination). This metric measures the proportion of variance in the target variable that is explained by the input features. R^2 was selected because it provides an intuitive understanding of model performance.

3.3.3 Model Development

3.3.3.1 Baseline Model Training

To establish a foundation for model development, training was initiated with simple, interpretable models such as Linear Regression and Decision Trees. These models help identify initial relationships between section thicknesses (sth1 to sth15) and target outcomes (e.g., Thermal Expansion).

3.3.3.2 Model Evaluation and Validation

Once baseline models were trained, their performance was evaluated using the test set. The primary focus during this phase was to identify the most promising models based on R^2 scores, guiding the selection for further refinement and tuning.

3.3.3.3 Iterative Feature Selection

To optimize model performance, an iterative feature selection process was employed, including:

- **Random Combination Testing:** This involved generating random subsets of section thickness features and training models on each subset. This approach allows for exploring different combinations and identifying those that yield the highest R^2 scores.
- **Correlation Filtering:** The correlation matrix for the thickness variables was calculated, removing pairs with high correlation (e.g., correlation coefficient > 0.8) to mitigate multicollinearity. This ensures that the selected features provide independent contributions to the model's predictive power.

3.3.3.4 Model Hyperparameter Tuning

To further enhance model performance, hyperparameter tuning was engaged for the selected models, such as AdaBoost and XGBoost. The objectives of this phase included identifying optimal configurations to improve model accuracy.

3.3.4 Advanced Techniques

3.3.4.1 Interaction Terms

To explore the potential impact of interactions between features, interaction terms among selected variables (e.g., sth2, sth3, sth4, sth5) were introduced. This approach is valuable because interaction terms can reveal complex relationships that individual features may not capture, potentially enhancing the model's explanatory power.

3.3.4.2 Rate of Change Terms

The rate of change terms for key thickness variables were also calculated to model dynamic trends in section thickness. This technique allows for capturing underlying patterns that may influence bottle performance, providing additional insights into how thickness variations impact outcomes.

3.3.5 Generalization across bottle types

The aim is to develop models that can generalize well across various bottle designs, particularly those with similar shapes. This is important because generalizable models provide broader applicability, enabling insights and predictions to be relevant for a range of related preforms. By avoiding overly specific models, the findings from this work can be used in future designs and improvements.

3.4 What-if analysis

The What-If Analysis is a tool that allows users to input values for input features (sth1 to sth15) for a specific bottle type to predict output variables (performance metrics). This scenario-based analysis helps forecast the impact of different bottle preform characteristics on performance metrics such as empty top load, burst expansion, burst pressure, and thermal expansion. It enables users to experiment with input values and understand their influence on bottle performance, making it essential for manufacturing optimization, quality control, and performance forecasting.

4. Results

4.1 Analysis of Best Models for each variable

To predict each target variable, a regression modeling approach was employed using thickness measurements from 15 bottle sections (sth1 to sth15) as input features. Initially, a variety of models, including Linear Regression, Decision Tree, Random Forest, and others, were tested on the full dataset. However, to improve each model, separate feature engineering was implemented.

4.1.1 Preform 1 (21.5g AXL bottle)

The predictive models for the 21.5g AXL bottle demonstrated excellent performance for the Empty Top Load and Burst Properties tests, achieving R^2 values exceeding 0.95 on the test set. In contrast, the Thermal Stability metrics showed varied outcomes. While Base Expansion and Lower Bumper Expansion achieved moderate accuracy ($R^2 \approx 0.50$), variables such as Upper Bumper Expansion and Lower Panel Expansion displayed lower predictability, with R^2 values below 0.35.

Test	Model Type	R2 (Train Test)
Upper Bumper Expansion	Linear Regression	0.33 0.32
Upper Panel Expansion	Random Forest	0.81 0.31
Mid Panel Expansion	Ada Boost	0.63 0.26
Lower Panel Expansion	Cat Boost	0.63 0.25
Lower Bumper Expansion	Ada Boost	0.61 0.50
Base Expansion	Extra Trees	0.96 0.55
Empty Top Load	Linear Regression	0.99 0.98
Burst Expansion	Linear Regression	0.99 0.98
Burst Pressure	Gradient Boosting	0.99 0.96

Table 4.1.1: 21.5g AXL Preform Best model Results

4.1.1.1 Upper Bumper Expansion

The best model for predicting Upper Bumper Expansion was Linear Regression. The selected features included individual thickness measurements (sth1, sth2, sth3, sth5, sth6, sth7, sth8, sth9, sth10, and sth15) along with interaction terms: $sth3 \times sth8 \times sth10$, $sth3 \times sth10$, $sth3 \times sth6 \times sth10$, $sth3 \times sth5 \times sth10$, $sth3 \times sth9 \times sth10$, and $sth3 \times sth8$. This model achieved an R^2 of 0.3267 on the training set and 0.3247 on the test set.

4.1.1.2 Upper Panel Expansion

The best-performing model for Upper Panel Expansion was the Random Forest algorithm. The features selected were sth1, sth4, sth10, sth13, and sth14. This model achieved an R^2 of 0.8128 on the training set but only 0.3112 on the test set, indicating potential overfitting.

4.1.1.3 Mid Panel Expansion

For Mid Panel Expansion, the AdaBoost algorithm performed best. It utilized all thickness features (sth1–sth15) with hyperparameters $n_estimators = 100$ and $random_state = 42$. The model achieved an R^2 of 0.6368 on the training set and 0.2551 on the test set.

4.1.1.4 Lower Panel Expansion

The CatBoost algorithm was the most effective model for Lower Panel Expansion. It used all thickness features (sth1–sth15) and was optimized with hyperparameters $iterations = 100$, $learning_rate = 0.1$, $depth = 3$, and $silent = True$. The model achieved an R^2 of 0.6346 on the training set and 0.2506 on the test set.

4.1.1.5 Lower Bumper Expansion

For Lower Bumper Expansion, the AdaBoost model was selected as the best-performing algorithm. It used all thickness features (sth1–sth15) and was fine-tuned with $n_estimators = 76$. This model delivered an R^2 of 0.606 on the training set and 0.496 on the test set.

4.1.1.6 Base Expansion

The Extra Trees algorithm was identified as the best model for Base Expansion. The selected features were sth4, sth7, sth12, sth13, and sth15. The model achieved an R^2 of 0.96 on the training set and 0.55 on the test set.

4.1.1.7 Empty Top Load

For predicting Empty Top Load, the Linear Regression using Lasso was chosen as the best model. It utilized all thickness features (sth1–sth15) and demonstrated excellent performance, with R^2 values of 0.9968 on the training set and 0.9813 on the test set.

4.1.1.8 Burst Expansion

The Linear Regression using Lasso model was also the best for predicting Burst Expansion. It employed all thickness features (sth1–sth15) and achieved R^2 values of 0.9988 on the training set and 0.9784 on the test set.

4.1.1.9 Burst Pressure

The Gradient Boosting algorithm was the most effective model for Burst Pressure. It utilized all thickness features (sth1–sth15) and was fine-tuned with $n_estimators = 134$. This model achieved R^2 values of 0.9995 on the training set and 0.9604 on the test set.

4.1.2 Preform 2 (20.5g AXL bottle)

The regression models for the 20.5g AXL bottle showed varying performance across the test variables. For the Burst Properties tests, the models performed well, with Burst Expansion and Burst Pressure achieving R^2 values of 0.97 and 0.94, respectively, indicating strong predictive capability. The Empty Top Load Test also demonstrated good performance, by achieving an R^2 value of 0.86 on the test set. Regarding the Thermal Stability tests, the models exhibited mixed results. While the Lower Bumper Expansion model showed relatively strong performance with an R^2 of 0.63, other metrics showed lower predictability with R^2 values ranging from 0.11 to 0.44, reflecting moderate to poor performance for these tests.

Test	Model Type	R2 (Train Test)
Upper Bumper Expansion	AdaBoost	0.80 0.30
Upper Panel Expansion	AdaBoost	0.59 0.34
Mid Panel Expansion	Gradient Boosting	0.90 0.44
Lower Panel Expansion	Random Forest	0.85 0.43
Lower Bumper Expansion	Decision Tree	1 0.57
Base Expansion	Random Forest	0.85 0.12
Empty Top Load	Linear Regression	0.87 0.86
Burst Expansion	Linear Regression	0.99 0.98
Burst Pressure	Gradient Boosting	0.99 0.94

Table 4.1.2: 20.5g AXL Preform Best model Results

4.1.2.1 Upper Bumper Expansion

The best model for predicting Upper Bumper Expansion was AdaBoost. Selected features included sth2, sth5, sth6, sth7, sth8, sth9, and sth15. The model was optimized with hyperparameters $n_estimators = 100$ and $random_state = 27$. It achieved an R^2 of 0.7972 on the training set and 0.2965 on the test set.

4.1.2.2 Upper Panel Expansion

The AdaBoost algorithm performed best for Upper Panel Expansion. Features selected were sth2, sth3, sth4, and sth5. The model used hyperparameters $n_estimators = 18$ and $random_state = 42$, achieving an R^2 of 0.5932 on the training set and 0.3373 on the test set.

4.1.2.3 Mid Panel Expansion

For Mid Panel Expansion, the Gradient Boosting model was the best performer. The selected features were sth10, sth12, and sth15. This model achieved an R^2 of 0.8995 on the training set and 0.4440 on the test set.

4.1.2.4 Lower Panel Expansion

The Random Forest algorithm was the top-performing model for Lower Panel Expansion. The features used were sth5, sth14, and sth6. This model delivered an R^2 of 0.8558 on the training set and 0.4316 on the test set.

4.1.2.5 Lower Bumper Expansion

For Lower Bumper Expansion, the Decision Tree model was identified as the best. The selected features were sth2, sth3, sth4, sth5, sth6, sth7, and sth8. The model was configured with the following hyperparameters:

criterion: squared_error, max_depth: None, max_features: None, max_leaf_nodes: None, min_samples_leaf: 1, min_samples_split: 2, random_state: 13, splitter: best

This model achieved an R^2 of 1.0 on the training set and 0.5665 on the test set.

4.1.2.6 Base Expansion

The Random Forest algorithm was the best choice for Base Expansion. Selected features included sth4, sth7, sth12, sth13, and sth15. The model achieved an R^2 of 0.8525 on the training set and 0.1184 on the test set.

4.1.2.7 Empty Top Load

For Empty Top Load prediction, the Linear Regression using Lasso model was the best performer. The features selected were sth4, sth6, sth7, sth11, sth12, sth13, and interaction terms: $sth1 \times sth2$, $sth2 \times sth3$, $sth2 \times sth15$, $sth4 \times sth11$, $sth4 \times sth15$, $sth5 \times sth6$, $sth6 \times sth7$, $sth6 \times sth13$, $sth7 \times sth11$, and $sth10 \times sth11$. This model achieved an R^2 of 0.8709 on the training set and 0.8603 on the test set.

4.1.2.8 Burst Expansion

The Linear Regression using Lasso model was also the best for Burst Expansion. It utilized all thickness features (sth1–sth15) and achieved R^2 values of 0.9982 on the training set and 0.9753 on the test set.

4.1.2.9 Burst Pressure

For Burst Pressure, the Gradient Boosting algorithm was the top-performing model. It used all thickness features (sth1–sth15) with the following hyperparameters:

alpha: 0.9, criterion: friedman_mse, learning_rate: 0.1, loss: squared_error, max_depth: 3, max_features: None, max_leaf_nodes: None, min_samples_leaf: 1, min_samples_split: 2, n_estimators: 100, subsample: 1.0, tol: 0.0001

The model achieved R^2 values of 0.9995 on the training set and 0.9348 on the test set.

4.1.3 Preform 3 (20.5g Ripples bottle DAK)

The regression models for the 20.5g DAK Ripples bottle demonstrated strong performance across most test variables. For the Thermal Stability tests, Upper Bumper Expansion, Upper Panel Expansion, Mid Panel Expansion, Lower Panel Expansion, Lower Bumper Expansion, and Panel Max Expansion showed excellent predictability, with R^2 values ranging from 0.92 to 0.98. However, the Base Expansion model performed less well, with an R^2 of 0.51. The Empty Top Load test showed moderate performance with an R^2 of 0.64. For the Burst Properties tests, both Burst Expansion and Burst Pressure demonstrated strong predictive capability, with R^2 values of 0.92 and 0.93, respectively.

Test	Model Type	R ² (Train Test)
Upper Bumper Expansion	Linear Regression	0.97 0.96
Upper Panel Expansion	Linear Regression	0.98 0.98
Mid Panel Expansion	Linear Regression	0.97 0.95
Lower Panel Expansion	Linear Regression	0.96 0.93
Lower Bumper Expansion	Linear Regression	0.97 0.94
Base Expansion	XG Boost	0.99 0.51
Panel Max Expansion	Linear Regression	0.98 0.95
Empty Top Load	XG Boost	1.0 0.64
Burst Expansion	Linear Regression	0.97 0.92
Burst Pressure	Cat Boost	0.99 0.93

Table 4.1.3: 20.5g Ripple DAK Preform Best model Results

4.1.3.1 Upper Bumper Expansion

The best model for Upper Bumper Expansion was Linear Regression using Lasso. This model selected a set of reciprocal squared features derived from section thickness values with a hyperparameter $\alpha = 0.01668$, the model achieved a train R² of 0.9668 and a test R² of 0.9537, demonstrating its strong predictive accuracy across both datasets.

4.1.3.2 Upper Panel Expansion

For Upper Panel Expansion, the best model was Linear Regression using Lasso. The selected features included a combination of reciprocal and reciprocal squared terms, using a hyperparameter $\alpha = 0.00464$, the model produced a train R² of 0.9842 and a test R² of 0.9770, reflecting excellent performance and generalization.

4.1.3.3 Mid Panel Expansion

The Mid Panel Expansion was best predicted using Linear Regression with Lasso, with features derived exclusively from the reciprocal squared thickness values: $1/sth1^2$ through $1/sth15^2$. The optimized hyperparameter $\alpha = 0.01668$ resulted in a train R^2 of 0.9725 and a test R^2 of 0.9544, demonstrating the model's strong predictive capability and reliability across datasets.

4.1.3.4 Lower Panel Expansion

The Lower Panel Expansion model also employed Linear Regression using Lasso, with the same reciprocal squared features as the Mid Panel Expansion model: $1/sth1^2$ through $1/sth15^2$. By using the optimized hyperparameter $\alpha = 0.01668$, the model achieved a train R^2 of 0.9641 and a test R^2 of 0.9368, confirming its strong predictive performance.

4.1.3.5 Lower Bumper Expansion

The best model for Lower Bumper Expansion was Linear Regression using Lasso. The model used a combination of reciprocal squared features, using a hyperparameter $\alpha = 0.01668$, the model achieved a train R^2 of 0.9693 and a test R^2 of 0.9402, indicating robust performance.

4.1.3.6 Base Expansion

The Base Expansion was best modeled using XGBoost, leveraging all section thickness values (sth1 through sth15) as features. The model achieved a train R^2 of 0.9986, reflecting near-perfect fit on the training data, but the test R^2 of 0.5155 indicated significant overfitting, highlighting the need for additional optimization to improve generalization.

4.1.3.7 Panel Max Expansion

The Panel Max Expansion was effectively predicted using Linear Regression with Lasso, utilizing reciprocal squared features across all thickness levels: $1/sth1^2$ through $1/sth15^2$. The model, with a hyperparameter $\alpha = 0.00464$, achieved a train R^2 of 0.9757 and a test R^2 of 0.9504, demonstrating its strong predictive capabilities and robustness.

4.1.3.8 Empty Top Load

For Empty Top Load, the best model was XGBoost, which utilized all section thickness values (sth1 through sth15) as input features. While the model achieved a train R^2 of 1.0000, indicating a perfect fit on training data, the test R^2 of 0.6374 pointed to overfitting, suggesting further refinement is necessary for improved generalization.

4.1.3.9 Burst Expansion

The Burst Expansion was best modeled using Linear Regression with Lasso, which utilized all section thickness values (sth1 through sth15) as features. The model exhibited strong performance, achieving a train R^2 of 0.9674 and a test R^2 of 0.9203, indicating high reliability and generalizability.

4.1.3.10 Burst Pressure

The best model for Burst Pressure was Cat Boost, which used all thickness values (sth1 through sth15) as input features. The model's hyperparameters—depth: 3, iterations: 100, l2_leaf_reg: 3, learning_rate: 0.2, and subsample: 0.8—were fine-tuned to optimize performance. As a result, the model achieved a train R^2 of 0.9911 and a test R^2 of 0.9281, showcasing exceptional predictive performance and generalization.

4.1.4 Preform 4 (20.5g Ripples bottle FENC)

Similar to the 20.5g Ripples bottle (DAK), the models for the Thermal Stability tests (Upper Bumper Expansion, Upper Panel Expansion, Mid Panel Expansion, Lower Panel Expansion, Lower Bumper Expansion, and Panel Max Expansion) performed well, but the Base Expansion and Empty Top Load tests exhibited more moderate predictive power.

Test	Model Type	R2 (Train Test)
Upper Bumper Expansion	Linear Regression	0.98 0.95
Upper Panel Expansion	Linear Regression	0.98 0.95
Mid Panel Expansion	Linear Regression	0.97 0.94
Lower Panel Expansion	Linear Regression	0.97 0.87
Lower Bumper Expansion	Linear Regression	0.95 0.83
Base Expansion	Random Forest	0.99 0.80
Panel Max Expansion	Linear Rgression	0.97 0.88
Empty Top Load	Catboost	0.99 0.77

Table 4.1.4: 20.5g Ripple FENC Preform Best model Results

4.1.4.1 Upper Bumper Expansion

The best model for Upper Bumper Expansion was Linear Regression using Lasso, leveraging a specific set of reciprocal squared features, using a hyperparameter $\alpha = 0.01668$, the model achieved a train R^2 of 0.9758 and a test R^2 of 0.9478, demonstrating high accuracy and robust performance across datasets.

4.1.4.2 Upper Panel Expansion

The best model for Upper Panel Expansion was also Linear Regression using Lasso, utilizing a comprehensive set of reciprocal squared features. The model achieved a train R^2 of 0.9836 and a test R^2 of 0.9523, reflecting excellent predictive performance.

4.1.4.3 Mid Panel Expansion

For Mid Panel Expansion, the best model was Linear Regression using Ridge, utilizing all thickness features (sth1 to sth30) and modulus features (mod1 to mod30). With a hyperparameter $\alpha = 0.01668$, the model achieved a train R^2 of 0.9726 and a test R^2 of 0.9461, demonstrating effective generalization.

4.1.4.4 Lower Panel Expansion

The best model for Lower Panel Expansion was Linear Regression using Lasso, selecting a broad range of reciprocal squared features. The hyperparameter $\alpha = 0.01668$ resulted in a train R^2 of 0.9737 and a test R^2 of 0.8698, indicating solid predictive performance, albeit with room for improvement in generalization.

4.1.4.5 Lower Bumper Expansion

For Lower Bumper Expansion, the best model was Linear Regression using Lasso, with selected features. The model achieved a train R^2 of 0.9456 and a test R^2 of 0.8342, indicating good predictive accuracy but room for improvement.

4.1.4.6 Base Expansion

The best model for Base Expansion was Random Forest, using all thickness features (sth1 to sth15). The model achieved a train R^2 of 0.9866 and a test R^2 of 0.8033, suggesting strong performance with some overfitting that could be mitigated through further tuning.

4.1.4.7 Panel Max Expansion

For Panel Max Expansion, the best model was Linear Regression using Ridge, leveraging all thickness (sth1 to sth30) and modulus (mod1 to mod30) features. With hyperparameters K-folds

=3, ridge_α = 1, and ridge_fit_intercept = True, the model achieved a train R² of 0.9700 and a test R² of 0.8822, reflecting robust predictive performance.

4.1.4.8 Empty Top Load

The best model for Empty Top Load was Cat Boost, using all thickness features (sth1 to sth15) and modulus features (mod1 to mod30). The model achieved an almost perfect train R² of 0.9999, but the test R² of 0.7723 highlighted overfitting, requiring further optimization for improved generalization.

4.2 Standard Models

The final Random Forest model for thermal expansion and the Linear Regression (Lasso) model for top load and burst properties were retrained on the full dataset using the optimal hyperparameters. The models were validated on a holdout test set, confirming their accuracy and generalization capabilities.

Test Variable	Model Type	21.5g (AXL)	20.5g (AXL)	20.5g (Ripple DAK)	20.5g (Ripple FENC)
Upper Bumper Expansion	Random Forest	0.57 0.44	0.45 0.13	0.99 0.96	0.99 0.92
Upper Panel Expansion		0.56 0.30	0.53 0.14	0.99 0.97	0.99 0.91
Mid Panel Expansion		0.55 0.29	0.10 0.01	0.96 0.94	0.99 0.81
Lower Panel Expansion		0.41 0.25	0.09 0.02	0.98 0.86	0.84 0.70
Lower Bumper Expansion		0.75 0.52	0.86 0.14	0.98 0.85	0.98 0.72
Base Expansion		0.75 0.33	0.27 -0.05	0.28 0.20	0.95 0.53
Panel Max Expansion		-	-	0.97 0.71	0.98 0.73
Empty Top Load	Linear Regression	0.99 0.98	0.87 0.86	0.65 0.50	0.78 0.51
Burst Expansion	Linear Regression	0.99 0.98	0.99 0.99	0.97 0.92	-
Burst Pressure		0.97 0.93	0.98 0.98	0.97 0.95	-

Table 4.2: Standard model results for all Preforms

Burst Expansion models show excellent performance ($R^2 > .90$ for both train and test), across all bottle types, demonstrating high consistency in predictions for this feature. While Random Forest models excel in some categories, particularly for Lower Panel Expansion, Linear Regression models with regularization offer strong performance in metrics like Empty Top Load and Burst Expansion.

4.2.1 Thermal Stability Test

4.2.1.1 Analysis

The thermal expansion test was conducted to identify the critical section thicknesses (Sth values) that significantly impact the performance of preforms under thermal stress. A standardized Random Forest Model was used to assess the importance of various thickness parameters (Sth1 to Sth8) across different bottle regions and expansion metrics.

4.2.1.2 Observations

The key findings from the analysis are as follows:

- **Upper Bumper and Upper Panel Expansions:** Sth3 and Sth5 were identified as the most significant contributors, with notable influence on thermal expansion behavior. Sth2 also played a role, albeit less prominently.
- **Middle and Lower Panel Expansions:** Sth2 and Sth3 emerged as dominant factors across all bottle types tested.
- **Base Expansion:** Both Sth3 and Sth5 demonstrated high importance in maintaining base structural integrity during thermal expansion.
- **Panel Max Expansion:** Sth4 showed a marked increase in significance alongside Sth2, highlighting its role in accommodating maximal panel deformation under thermal stress.

4.2.2 Empty Top Load Test

4.2.2.1 Analysis

The Empty Top Load Test was conducted to evaluate the structural integrity of bottles under top-load stress when empty. The analysis focused on identifying critical section thickness values (Sth) that influence the bottle's ability to withstand compressive forces without deforming.

The study examined four different preform types (AXL 20.5g, AXL 21.5g, Ripple DAK 20.5g, and Ripple FENC 20.5g) to determine the key performance indicators (KPIs) affecting top-load performance.

4.2.2.2 Observations

Across all preform types, the Grip and Shoulder sections were identified as the most critical regions.

The following section thicknesses were ranked as top contributors for each preform:

Preform Type	Top KPI
AXL 20.5g	Sth13, Sth15, Sth2, Sth12, Sth7
AXL 21.5g	Sth13, Sth7, Sth2, Sth14
Ripple DAK 20.5g	Sth11, Sth8, Sth14, Sth5
Ripple FENC 20.5g	Sth10, Sth1, Sth5, Sth12

Table 4.2.2.2: Top Features for Empty Top Load Test

A decrease in thickness in one section leads to increased stress on adjacent areas. Proper material distribution in the Grip and Shoulder sections is vital to prevent structural weakness while maintaining the overall performance of other areas.

4.2.3 Burst Properties

4.2.3.1 Analysis

Burst Properties test was conducted by observing burst expansion and burst pressure values. The analysis focused on identifying critical section thickness values (Sth) that influence the bottle's ability to withstand compressive forces without deforming. The study examined four different preform types (AXL 20.5g, AXL 21.5g, Ripple DAK 20.5g, and Ripple FENC 20.5g) to determine the key performance indicators (KPIs) affecting Burst performance.

4.2.3.2 Observations

For Burst Pressure and Burst Expansion, the thicknesses at Label and Grip sections play the most important role. So, it is crucial to ensure sufficient thickness throughout the entire bottle to meet the criteria for both burst pressure and expansion.

Preform Type	Top KPI Burst Pressure	Top KPI Burst Expansion
AXL 20.5g	Sth15, Sth11, Sth2, Sth13, Sth14	Sth3, Sth11, Sth15, Sth13, Sth4
AXL 21.5g	Sth7, Sth8, Sth10, Sth2, Sth11	Sth5, Sth10, Sth3, Sth11, Sth10
Ripple DAK 20.5g	Sth15, Sth6, Sth11, Sth14, Sth1	Sth6, Sth15, Sth4, Sth11, Sth11

Table 4.2.3.2: Top Features for Burst Properties Test

5. Conclusions and Recommendations

The analysis highlights the importance of optimizing material distribution to improve bottle performance while aligning with sustainability goals. Key findings demonstrate the critical role of sections Sth2, Sth3, Sth4, and Sth5 in enhancing thermal performance across various bottle types and expansion metrics. Balancing the thickness of these sections can significantly reduce material usage without compromising structural integrity.

In the context of Empty Top Load performance, the grip and shoulder sections emerged as the most sensitive to compressive stresses. Managing their thickness optimally prevents premature failure and ensures a balance between structural integrity and material efficiency. Achieving this balance enhances bottle performance across varying loading conditions while maintaining critical functionality.

5.1 Optimizing Bottle Performance through ML and Traditional Testing Methods

A hybrid approach combining Machine Learning (ML) models with traditional testing methods proves most effective for optimizing bottle design. The analysis underscores the differences in performance across bottle types, metrics, and testing conditions, necessitating a mixed methodology to ensure accuracy and reliability.

5.1.1 Thermal Expansion Performance

For Ripple bottles, ML models demonstrated superior predictive capability in assessing thermal expansion behavior, enabling accurate design optimizations based on material properties. Conversely, AXL bottles showed lower prediction accuracy in thermal models, necessitating validation through traditional testing to ensure safety and reliability.

5.1.2 Top Load Performance

ML models effectively predicted Empty Top Load performance for AXL bottles, streamlining the optimization process. However, this capability was not mirrored in Ripple bottles, where traditional testing remains essential to meet safety standards.

5.1.3 Burst Expansion and Burst Test

For both AXL and Ripple bottles, ML models consistently excelled in predicting burst expansion and burst test metrics. This reliability eliminates the need for extensive physical testing in this domain, allowing for efficient performance assessments across various bottle designs.

5.1.4 Hybrid Approach:

The mixed performance of ML models across different metrics suggests adopting a hybrid approach:

- ML models should be applied for metrics where strong predictive capabilities were observed, such as thermal expansion for Ripple bottles, top load for AXL bottles, and burst testing for all bottle types.
- Traditional testing methods should complement ML models in areas with weaker predictive accuracy, such as thermal expansion for AXL bottles and top load for Ripple bottles.

This combination leverages the strengths of both methodologies, enabling streamlined testing, cost reduction, and optimized product performance without compromising safety or quality.

5.2 Performance Optimization and Material Selection for AXL and Ripple Bottles

The evaluation of AXL and Ripple bottles provided valuable insights into performance and material selection.

5.2.1 AXL Bottles

For AXL bottles, the 21.5g bottle was found to be overengineered, with no thermal failures observed. This suggests that the additional material may be unnecessary. The 20.5g bottle, while exhibiting some thermal failures, performed within safe limits for most metrics. This indicates that the 20.5g AXL bottle can be further optimized to eliminate these failures while significantly reducing plastic usage. Such optimization aligns with PepsiCo's pep+ sustainability initiative, promoting resource efficiency without compromising performance.

5.2.2 Ripple Bottles

For Ripple bottles, material analysis revealed that FENC outperforms DAK in thermal performance. FENC-based bottles exhibit lower thermal expansion at the same thickness, making them more structurally reliable under thermal stress. Adopting FENC for Ripple bottles enhances their durability and performance, while also reducing the likelihood of thermal failures.

6. References

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7. Appendix

This appendix includes the detailed linear regression equations derived for predicting various bottle performance metrics, such as Upper Bumper Expansion, Upper Panel Expansion, Lower Panel Expansion, and Lower Bumper Expansion. These equations represent the relationship between the selected features and the corresponding performance metric as determined by the best-fit Linear Regression models.

7.1 Upper Bumper Expansion Ripple DAK

The Linear Regression equation for predicting Upper Bumper Expansion for Ripple DAK Bottle is as follows:

$$Y = 0.3021 + (0.0003 * 1/sth1^2_x_1/sth2^2) + (0.0005 * 1/sth1^2_x_1/sth3^2) + (-0.0001 * 1/sth1^2_x_1/sth7^2) + (-0.0000 * 1/sth1^2_x_1/sth10^2) + (-0.0000 * 1/sth1^2_x_1/sth15^2) + (-0.0002 * 1/sth2^2_x_1/sth8^2) + (-0.0002 * 1/sth2^2_x_1/sth10^2) + (-0.0001 * 1/sth2^2_x_1/sth15^2) + (0.0004 * 1/sth3^2_x_1/sth6^2) + (0.0000 * 1/sth3^2_x_1/sth13^2) + (0.0000 * 1/sth3^2_x_1/sth14^2) + (0.0000 * 1/sth3^2_x_1/sth15^2) + (0.0002 * 1/sth6^2_x_1/sth7^2) + (0.0002 * 1/sth6^2_x_1/sth15^2) + (-0.0000 * 1/sth12^2_x_1/sth13^2) + (-0.0000 * 1/sth13^2_x_1/sth14^2)$$

7.2 Upper Bumper Expansion Ripple FENC

The Linear Regression equation for predicting Upper Bumper Expansion for Ripple FENC Bottle is as follows:

$$Y = 0.2209 + (0.0002 * 1/sth1^2_x_1/sth2^2) + (0.0003 * 1/sth1^2_x_1/sth4^2) + (0.0002 * 1/sth1^2_x_1/sth7^2) + (-0.0001 * 1/sth1^2_x_1/sth23^2) + (-0.0001 * 1/sth1^2_x_1/sth25^2) + (0.0001 * 1/sth2^2_x_1/sth4^2) + (-0.0000 * 1/sth2^2_x_1/sth30^2) + (-0.0001 * 1/sth3^2_x_1/sth25^2) + (-0.0000 * 1/sth3^2_x_1/sth26^2) + (-0.0001 * 1/sth3^2_x_1/sth30^2) + (0.0002 * 1/sth4^2_x_1/sth7^2) + (0.0002 * 1/sth4^2_x_1/sth14^2) + (0.0001 * 1/sth4^2_x_1/sth24^2) + (0.0001 * 1/sth4^2_x_1/sth29^2) + (0.0001 * 1/sth13^2_x_1/sth14^2) + (0.0000 * 1/sth14^2_x_1/sth15^2) + (-0.0000 * 1/sth19^2_x_1/sth29^2) + (-0.0000 * 1/sth23^2_x_1/sth28^2) + (-0.0001 * 1/sth23^2_x_1/sth29^2) + (0.0000 * 1/sth25^2_x_1/sth26^2) + (0.0000 * 1/sth25^2_x_1/sth27^2) + (0.0000 * 1/sth25^2_x_1/sth30^2) + (-0.0000 * 1/sth26^2_x_1/sth28^2) + (-0.0000 * 1/sth26^2_x_1/sth29^2)$$

7.3 Upper Panel Expansion Ripple DAK

The Linear Regression equation for predicting Upper Panel Expansion for Ripple DAK Bottle is as follows:

$$Y = 1.6985 + (0.0047 * 1/sth1_x_1/sth1^2) + (0.0004 * 1/sth1^2_x_1/sth2^2) + (0.0009 * 1/sth1^2_x_1/sth3^2) + (-0.0006 * 1/sth1^2_x_1/sth5^2) + (-0.0001 * 1/sth1^2_x_1/sth6^2) + (-0.0001 * 1/sth1^2_x_1/sth8^2) + (-0.0005 * 1/sth1^2_x_1/sth9^2) + (-0.0005 * 1/sth1^2_x_1/sth10^2) + (-0.0016 * 1/sth1^2_x_1/sth11^2) + (0.0001 * 1/sth1^2_x_1/sth12^2) + (0.0001 * 1/sth1^2_x_1/sth13^2) + (0.0000 * 1/sth1^2_x_1/sth14^2) + (-0.0000 * 1/sth1^2_x_1/sth15^2) + (-0.0002 * 1/sth2^2_x_1/sth3^2) + (-0.0000 * 1/sth2^2_x_1/sth5^2) + (-0.0003 * 1/sth2^2_x_1/sth9^2) + (-0.0001 * 1/sth2^2_x_1/sth13^2) + (-0.0001 * 1/sth2^2_x_1/sth15^2) + (0.0001 * 1/sth3^2_x_1/sth12^2) + (0.0004 * 1/sth3^2_x_1/sth13^2) + (0.0003 * 1/sth3^2_x_1/sth14^2) + (0.0001 * 1/sth4^2_x_1/sth6^2) + (0.0001 * 1/sth4^2_x_1/sth12^2) + (0.0001 * 1/sth4^2_x_1/sth14^2) + (0.0002 * 1/sth4^2_x_1/sth15^2) + (0.0010 * 1/sth6^2_x_1/sth7^2) + (0.0005 * 1/sth6^2_x_1/sth9^2) + (0.0012 * 1/sth6^2_x_1/sth11^2) + (0.0001 * 1/sth6^2_x_1/sth15^2) + (0.0002 * 1/sth7^2_x_1/sth9^2) + (-0.0002 * 1/sth7^2_x_1/sth13^2) + (-0.0003 * 1/sth7^2_x_1/sth14^2) + (-0.0001 * 1/sth8^2_x_1/sth14^2) + (0.0001 * 1/sth11^2_x_1/sth12^2) + (0.0000 * 1/sth11^2_x_1/sth13^2) + (-0.0002 * 1/sth12^2_x_1/sth13^2) + (0.0000 * 1/sth12^2_x_1/sth15^2) + (0.0000 * 1/sth13^2_x_1/sth14^2) + (-0.0000 * 1/sth13^2_x_1/sth15^2)$$

7.4 Upper Panel Expansion Ripple FENC

The Linear Regression equation for predicting Upper Panel Expansion for Ripple FENC Bottle is as follows:

$$Y = 1.5439 + (0.0004 * 1/sth1^2_x_1/sth2^2) + (0.0003 * 1/sth1^2_x_1/sth4^2) + (0.0000 * 1/sth1^2_x_1/sth5^2) + (0.0005 * 1/sth1^2_x_1/sth7^2) + (-0.0002 * 1/sth1^2_x_1/sth23^2) + (-0.0002 * 1/sth1^2_x_1/sth25^2) + (-0.0001 * 1/sth1^2_x_1/sth27^2) + (0.0000 * 1/sth2^2_x_1/sth4^2) + (-0.0000 * 1/sth3^2_x_1/sth25^2) + (-0.0000 * 1/sth3^2_x_1/sth26^2) + (-0.0001 * 1/sth3^2_x_1/sth30^2) + (0.0002 * 1/sth4^2_x_1/sth7^2) + (0.0005 * 1/sth4^2_x_1/sth29^2) + (0.0002 * 1/sth5^2_x_1/sth14^2) + (0.0001 * 1/sth5^2_x_1/sth24^2) + (0.0000 * 1/sth5^2_x_1/sth28^2) + (0.0000 * 1/sth7^2_x_1/sth14^2) + (0.0005 * 1/sth7^2_x_1/sth28^2) + (0.0001 * 1/sth12^2_x_1/sth14^2) + (0.0000 * 1/sth13^2_x_1/sth26^2) + (0.0000 * 1/sth14^2_x_1/sth24^2) + (0.0000 * 1/sth14^2_x_1/sth25^2) + (0.0001 * 1/sth14^2_x_1/sth26^2) + (0.0002 * 1/sth15^2_x_1/sth23^2) + (0.0000 * 1/sth15^2_x_1/sth24^2)$$

$$\begin{aligned}
& + (-0.0001 * 1/sth18^2_x_1/sth29^2) + (-0.0001 * 1/sth18^2_x_1/sth30^2) + (-0.0000 * \\
& 1/sth19^2_x_1/sth29^2) + (0.0000 * 1/sth20^2_x_1/sth23^2) + (0.0000 * 1/sth20^2_x_1/sth24^2) \\
& + (0.0000 * 1/sth20^2_x_1/sth25^2) + (0.0000 * 1/sth20^2_x_1/sth26^2) + (0.0000 * \\
& 1/sth20^2_x_1/sth27^2) + (-0.0000 * 1/sth23^2_x_1/sth25^2) + (-0.0001 * \\
& 1/sth23^2_x_1/sth29^2) + (-0.0000 * 1/sth24^2_x_1/sth29^2) + (0.0000 * \\
& 1/sth25^2_x_1/sth26^2) + (0.0000 * 1/sth25^2_x_1/sth27^2) + (0.0000 * 1/sth25^2_x_1/sth30^2) \\
& + (-0.0000 * 1/sth26^2_x_1/sth29^2) + (-0.0000 * 1/sth27^2_x_1/sth29^2)
\end{aligned}$$

7.5 Mid Panel DAK

The Linear Regression equation for predicting Mid Panel Expansion for Ripple DAK Bottle is as follows:

$$\begin{aligned}
Y = & 1.7334 + (0.0004 * 1/sth1^2_x_1/sth2^2) + (0.0009 * 1/sth1^2_x_1/sth3^2) + (-0.0004 * \\
& 1/sth1^2_x_1/sth7^2) + (-0.0000 * 1/sth1^2_x_1/sth8^2) + (-0.0003 * 1/sth1^2_x_1/sth10^2) + (- \\
& 0.0001 * 1/sth1^2_x_1/sth11^2) + (-0.0003 * 1/sth2^2_x_1/sth8^2) + (-0.0000 * \\
& 1/sth2^2_x_1/sth9^2) + (-0.0002 * 1/sth2^2_x_1/sth15^2) + (0.0002 * 1/sth3^2_x_1/sth13^2) + \\
& (0.0001 * 1/sth4^2_x_1/sth6^2) + (0.0002 * 1/sth4^2_x_1/sth12^2) + (0.0001 * \\
& 1/sth4^2_x_1/sth13^2) + (0.0001 * 1/sth4^2_x_1/sth14^2) + (0.0004 * 1/sth5^2_x_1/sth6^2) + \\
& (0.0008 * 1/sth6^2_x_1/sth7^2) + (0.0006 * 1/sth6^2_x_1/sth15^2) + (-0.0001 * \\
& 1/sth12^2_x_1/sth13^2) + (-0.0000 * 1/sth13^2_x_1/sth14^2) + (-0.0001 * \\
& 1/sth13^2_x_1/sth15^2)
\end{aligned}$$

7.6 Lower Panel DAK

The Linear Regression equation for predicting Lower Panel Expansion for Ripple DAK Bottle is as follows:

$$\begin{aligned}
Y = & 1.8049 + (0.0004 * 1/sth1^2_x_1/sth2^2) + (0.0008 * 1/sth1^2_x_1/sth3^2) + (-0.0003 * \\
& 1/sth1^2_x_1/sth7^2) + (-0.0003 * 1/sth1^2_x_1/sth10^2) + (-0.0000 * 1/sth1^2_x_1/sth11^2) + \\
& (-0.0000 * 1/sth1^2_x_1/sth15^2) + (-0.0000 * 1/sth2^2_x_1/sth8^2) + (-0.0003 * \\
& 1/sth2^2_x_1/sth15^2) + (-0.0002 * 1/sth4^2_x_1/sth15^2) + (0.0008 * 1/sth6^2_x_1/sth7^2) + \\
& (0.0002 * 1/sth6^2_x_1/sth12^2) + (0.0003 * 1/sth6^2_x_1/sth13^2) + (0.0000 * \\
& 1/sth6^2_x_1/sth14^2) + (0.0009 * 1/sth6^2_x_1/sth15^2) + (-0.0000 * 1/sth8^2_x_1/sth15^2) + \\
& (-0.0000 * 1/sth10^2_x_1/sth13^2) + (-0.0001 * 1/sth12^2_x_1/sth13^2) + (-0.0001 * \\
& 1/sth13^2_x_1/sth15^2)
\end{aligned}$$

7.7 Lower Panel FENC

The Linear Regression equation for predicting Lower Panel Expansion for Ripple FENC Bottle is as follows:

$$Y = 1.2058 + (0.0001 * 1/sth1^2_x_1/sth2^2) + (0.0004 * 1/sth1^2_x_1/sth4^2) + (0.0002 * 1/sth1^2_x_1/sth7^2) + (0.0000 * 1/sth1^2_x_1/sth14^2) + (0.0000 * 1/sth2^2_x_1/sth4^2) + (0.0000 * 1/sth2^2_x_1/sth14^2) + (-0.0001 * 1/sth2^2_x_1/sth27^2) + (-0.0001 * 1/sth2^2_x_1/sth30^2) + (-0.0001 * 1/sth3^2_x_1/sth25^2) + (0.0002 * 1/sth4^2_x_1/sth7^2) + (0.0003 * 1/sth4^2_x_1/sth14^2) + (0.0000 * 1/sth4^2_x_1/sth29^2) + (0.0001 * 1/sth5^2_x_1/sth13^2) + (0.0000 * 1/sth7^2_x_1/sth29^2) + (0.0002 * 1/sth12^2_x_1/sth13^2) + (0.0000 * 1/sth12^2_x_1/sth24^2) + (0.0002 * 1/sth12^2_x_1/sth25^2) + (0.0002 * 1/sth12^2_x_1/sth26^2) + (0.0007 * 1/sth13^2_x_1/sth14^2) + (0.0003 * 1/sth13^2_x_1/sth15^2) + (0.0002 * 1/sth13^2_x_1/sth16^2) + (0.0001 * 1/sth13^2_x_1/sth24^2) + (0.0001 * 1/sth13^2_x_1/sth25^2) + (0.0002 * 1/sth13^2_x_1/sth26^2) + (0.0000 * 1/sth13^2_x_1/sth27^2) + (0.0001 * 1/sth15^2_x_1/sth23^2) + (0.0001 * 1/sth15^2_x_1/sth24^2) + (0.0000 * 1/sth15^2_x_1/sth25^2) + (0.0001 * 1/sth15^2_x_1/sth26^2) + (0.0000 * 1/sth15^2_x_1/sth27^2) + (0.0000 * 1/sth16^2_x_1/sth24^2) + (0.0001 * 1/sth16^2_x_1/sth25^2) + (0.0000 * 1/sth16^2_x_1/sth26^2) + (0.0000 * 1/sth16^2_x_1/sth27^2) + (-0.0000 * 1/sth18^2_x_1/sth26^2) + (-0.0000 * 1/sth18^2_x_1/sth29^2) + (-0.0000 * 1/sth22^2_x_1/sth24^2) + (-0.0001 * 1/sth22^2_x_1/sth25^2) + (-0.0000 * 1/sth22^2_x_1/sth26^2) + (-0.0000 * 1/sth23^2_x_1/sth24^2) + (-0.0001 * 1/sth23^2_x_1/sth25^2) + (-0.0000 * 1/sth23^2_x_1/sth26^2) + (-0.0001 * 1/sth23^2_x_1/sth29^2) + (-0.0000 * 1/sth24^2_x_1/sth29^2) + (0.0000 * 1/sth25^2_x_1/sth27^2) + (0.0000 * 1/sth25^2_x_1/sth28^2)$$

7.8 Panel Max DAK

The Linear Regression equation for predicting Panel Max Expansion for Ripple DAK Bottle is as follows:

$$Y = 1.9468 + (0.0003 * 1/sth1^2_x_1/sth2^2) + (0.0007 * 1/sth1^2_x_1/sth3^2) + (-0.0002 * 1/sth1^2_x_1/sth10^2) + (-0.0012 * 1/sth1^2_x_1/sth11^2) + (0.0003 * 1/sth1^2_x_1/sth13^2) + (-0.0000 * 1/sth1^2_x_1/sth15^2) + (-0.0000 * 1/sth2^2_x_1/sth3^2) + (-0.0000 * 1/sth2^2_x_1/sth5^2) + (-0.0001 * 1/sth2^2_x_1/sth13^2) + (-0.0001 * 1/sth2^2_x_1/sth15^2) + (-0.0001 * 1/sth3^2_x_1/sth5^2) + (0.0004 * 1/sth3^2_x_1/sth12^2) + (0.0000 * 1/sth3^2_x_1/sth13^2) + (0.0001 * 1/sth3^2_x_1/sth14^2) + (-0.0003 * 1/sth4^2_x_1/sth5^2) +$$

$$\begin{aligned}
& (-0.0001 * 1/sth4^2_x_1/sth15^2) + (-0.0004 * 1/sth5^2_x_1/sth13^2) + (-0.0003 * \\
& 1/sth5^2_x_1/sth15^2) + (0.0014 * 1/sth6^2_x_1/sth7^2) + (0.0005 * 1/sth6^2_x_1/sth8^2) + \\
& (0.0001 * 1/sth6^2_x_1/sth9^2) + (0.0011 * 1/sth6^2_x_1/sth11^2) + (0.0002 * \\
& 1/sth6^2_x_1/sth12^2) + (0.0007 * 1/sth6^2_x_1/sth13^2) + (0.0001 * 1/sth6^2_x_1/sth14^2) + \\
& (0.0008 * 1/sth6^2_x_1/sth15^2) + (-0.0002 * 1/sth7^2_x_1/sth13^2) + (-0.0002 * \\
& 1/sth7^2_x_1/sth14^2) + (-0.0001 * 1/sth8^2_x_1/sth14^2) + (-0.0000 * 1/sth9^2_x_1/sth15^2) + \\
& (0.0000 * 1/sth11^2_x_1/sth12^2) + (0.0001 * 1/sth11^2_x_1/sth13^2) + (-0.0003 * \\
& 1/sth12^2_x_1/sth13^2) + (0.0001 * 1/sth12^2_x_1/sth15^2) + (-0.0000 * \\
& 1/sth13^2_x_1/sth14^2) + (-0.0000 * 1/sth13^2_x_1/sth15^2)
\end{aligned}$$

7.9 Panel Max FENC

The Linear Regression equation for predicting Panel Max Expansion for Ripple FENC Bottle is as follows:

$$\begin{aligned}
Y = & 2.5801 + (-0.0088 * sth1) + (0.0110 * sth2) + (0.0033 * sth3) + (-0.0170 * sth4) + (-0.0058 * \\
& sth5) + (0.0028 * sth6) + (0.0022 * sth7) + (0.0190 * sth8) + (-0.0027 * sth9) + (-0.0176 * sth10) \\
& + (-0.0171 * sth11) + (-0.0171 * sth12) + (-0.0117 * sth13) + (-0.0068 * sth14) + (-0.0086 * sth15) \\
& + (0.0285 * mod1) + (0.0018 * mod2) + (-0.0035 * mod3) + (0.0480 * mod4) + (0.0095 * mod5) \\
& + (0.0079 * mod6) + (0.0002 * mod7) + (-0.0134 * mod8) + (-0.0032 * mod9) + (0.0025 * mod10) \\
& + (-0.0018 * mod11) + (-0.0023 * mod12) + (0.0055 * mod13) + (0.0067 * mod14) + (0.0059 * \\
& mod15) + (0.0147 * sth16) + (0.0123 * sth17) + (0.0207 * sth18) + (0.0082 * sth19) + (-0.0067 * \\
& sth20) + (-0.0144 * sth21) + (-0.0056 * sth22) + (0.0055 * sth23) + (-0.0077 * sth24) + (0.0067 * \\
& sth25) + (-0.0018 * sth26) + (-0.0099 * sth27) + (0.0026 * sth28) + (-0.0009 * sth29) + (0.0175 * \\
& sth30) + (0.0148 * mod16) + (0.0198 * mod17) + (0.0030 * mod18) + (0.0121 * mod19) + (0.0061 \\
& * mod20) + (-0.0032 * mod21) + (-0.0133 * mod22) + (-0.0106 * mod23) + (0.0007 * mod24) + \\
& (0.0033 * mod25) + (0.0005 * mod26) + (0.0084 * mod27) + (0.0038 * mod28) + (-0.0058 * \\
& mod29) + (0.0068 * mod30)
\end{aligned}$$

7.10 Lower Bumper Expansion DAK

The Linear Regression equation for predicting Lower Bumper Expansion for Ripple DAK Bottle is as follows:

$$\begin{aligned}
Y = & 1.3456 + (0.0004 * 1/sth1^2_x_1/sth2^2) + (0.0003 * 1/sth1^2_x_1/sth3^2) + (-0.0001 * \\
& 1/sth1^2_x_1/sth11^2) + (-0.0000 * 1/sth1^2_x_1/sth15^2) + (-0.0002 * 1/sth2^2_x_1/sth15^2) + \\
& (0.0002 * 1/sth3^2_x_1/sth12^2) + (0.0001 * 1/sth3^2_x_1/sth13^2) + (-0.0004 *
\end{aligned}$$

$$1/\text{sth4}^2_x_1/\text{sth15}^2) + (-0.0000 * 1/\text{sth5}^2_x_1/\text{sth15}^2) + (0.0010 * 1/\text{sth6}^2_x_1/\text{sth7}^2) + (0.0008 * 1/\text{sth6}^2_x_1/\text{sth8}^2) + (0.0001 * 1/\text{sth6}^2_x_1/\text{sth9}^2) + (0.0002 * 1/\text{sth6}^2_x_1/\text{sth12}^2) + (0.0001 * 1/\text{sth6}^2_x_1/\text{sth13}^2) + (0.0008 * 1/\text{sth6}^2_x_1/\text{sth15}^2) + (-0.0001 * 1/\text{sth12}^2_x_1/\text{sth13}^2) + (-0.0000 * 1/\text{sth12}^2_x_1/\text{sth14}^2) + (-0.0000 * 1/\text{sth13}^2_x_1/\text{sth14}^2)$$

7.11 Lower Bumper Expansion FENC

The Linear Regression equation for predicting Lower Bumper Expansion for Ripple FENC Bottle is as follows:

$$Y = -0.8519 + (0.0003 * 1/\text{sth1}^2_x_1/\text{sth2}^2) + (-0.0000 * 1/\text{sth1}^2_x_1/\text{sth15}^2) + (-0.0000 * 1/\text{sth1}^2_x_1/\text{sth17}^2) + (-0.0000 * 1/\text{sth1}^2_x_1/\text{sth24}^2) + (-0.0003 * 1/\text{sth1}^2_x_1/\text{sth29}^2) + (-0.0000 * 1/\text{sth1}^2_x_1/\text{sth30}^2) + (0.0001 * 1/\text{sth2}^2_x_1/\text{sth4}^2) + (0.0000 * 1/\text{sth2}^2_x_1/\text{sth7}^2) + (-0.0000 * 1/\text{sth3}^2_x_1/\text{sth15}^2) + (-0.0000 * 1/\text{sth3}^2_x_1/\text{sth17}^2) + (-0.0000 * 1/\text{sth3}^2_x_1/\text{sth21}^2) + (-0.0000 * 1/\text{sth3}^2_x_1/\text{sth24}^2) + (-0.0000 * 1/\text{sth3}^2_x_1/\text{sth29}^2) + (-0.0000 * 1/\text{sth3}^2_x_1/\text{sth30}^2) + (0.0002 * 1/\text{sth7}^2_x_1/\text{sth29}^2) + (0.0003 * 1/\text{sth13}^2_x_1/\text{sth25}^2) + (0.0001 * 1/\text{sth13}^2_x_1/\text{sth26}^2) + (0.0001 * 1/\text{sth13}^2_x_1/\text{sth27}^2) + (0.0000 * 1/\text{sth13}^2_x_1/\text{sth28}^2) + (0.0001 * 1/\text{sth13}^2_x_1/\text{sth29}^2) + (0.0000 * 1/\text{sth14}^2_x_1/\text{sth26}^2) + (0.0000 * 1/\text{sth14}^2_x_1/\text{sth27}^2) + (0.0000 * 1/\text{sth14}^2_x_1/\text{sth29}^2) + (0.0000 * 1/\text{sth14}^2_x_1/\text{sth30}^2) + (0.0000 * 1/\text{sth16}^2_x_1/\text{sth26}^2) + (0.0000 * 1/\text{sth16}^2_x_1/\text{sth28}^2) + (0.0000 * 1/\text{sth16}^2_x_1/\text{sth29}^2) + (-0.0000 * 1/\text{sth17}^2_x_1/\text{sth24}^2) + (-0.0000 * 1/\text{sth21}^2_x_1/\text{sth27}^2) + (-0.0001 * 1/\text{sth22}^2_x_1/\text{sth25}^2) + (-0.0001 * 1/\text{sth22}^2_x_1/\text{sth26}^2) + (-0.0002 * 1/\text{sth23}^2_x_1/\text{sth25}^2) + (-0.0000 * 1/\text{sth23}^2_x_1/\text{sth26}^2) + (-0.0000 * 1/\text{sth24}^2_x_1/\text{sth26}^2)$$

7.12 Burst Expansion - 20.5 AXL

The Linear Regression equation for predicting Burst Expansion for 20.5g AXL Bottle is as follows:

$$Y = -0.4422 * \text{sth3} + -0.4708 * \text{sth4} + -0.7609 * \text{sth5} + -0.0518 * \text{sth6} + -0.3470 * \text{sth7} + -0.1508 * \text{sth8} + -0.2561 * \text{sth10} + -0.2763 * \text{sth11} + -0.0150 * \text{sth12} + 0.2429 * 1/\text{sth1} + 0.0913 * 1/\text{sth3} + 0.1396 * 1/\text{sth4} + 0.0553 * 1/\text{sth5} + 0.0925 * 1/\text{sth6} + 0.2026 * 1/\text{sth7} + 0.1956 * 1/\text{sth8} + 0.2447 * 1/\text{sth10} + 0.2280 * 1/\text{sth11} + 0.0136 * 1/\text{sth12} + 0.2166 * 1/\text{sth13} + 0.0838 * 1/\text{sth15} + 0.0302 * \text{sth1} \text{ sth13} + -0.0223 * \text{sth1} \text{ 1/sth14} + -0.0338 * \text{sth2} \text{ 1/sth12} + -0.1056 * \text{sth3} \text{ 1/sth15} + -0.0909 * \text{sth4} \text{ sth11} + -0.0457 * \text{sth4} \text{ 1/sth3} + -0.0985 * \text{sth4} \text{ 1/sth4} + -0.0317 * \text{sth4} \text{ 1/sth12} + 0.1320 *$$

$$\begin{aligned} & \text{sth6}^2 + 0.0037 * \text{sth6 sth7} + -0.1903 * \text{sth6 1/sth3} + -0.0072 * \text{sth6 1/sth7} + -0.2542 * \text{sth7 1/sth4} \\ & + -0.0005 * \text{sth8 1/sth3} + -0.2497 * \text{sth9 sth10} + 0.0752 * \text{sth12 sth13} + -0.1391 * \text{sth12 1/sth1} + \\ & -0.1030 * \text{sth12 1/sth15} + 0.1442 * \text{sth13}^2 + 0.0638 * \text{sth14 1/sth4} + 0.0472 * \text{sth14 1/sth8} + - \\ & 0.1829 * \text{sth15 1/sth15} + 0.2239 * 1/\text{sth1}^2 + 0.0957 * 1/\text{sth1 1/sth8} + 0.0617 * 1/\text{sth3}^2 + 0.3744 \\ & * 1/\text{sth3 1/sth4} + 0.0017 * 1/\text{sth3 1/sth8} + 0.0248 * 1/\text{sth4 1/sth7} + 0.0023 * 1/\text{sth4 1/sth8} + 0.1613 \\ & * 1/\text{sth4 1/sth9} + 0.0428 * 1/\text{sth5 1/sth9} + 0.0050 * 1/\text{sth5 1/sth10} + 0.0029 * 1/\text{sth5 1/sth12} + \\ & 0.0170 * 1/\text{sth6 1/sth10} + 0.0834 * 1/\text{sth7 1/sth9} + 0.3619 * 1/\text{sth7 1/sth10} + 0.1499 * 1/\text{sth7} \\ & 1/\text{sth15} + 0.0062 * 1/\text{sth8}^2 + 0.5041 * 1/\text{sth10}^2 + 0.1142 * 1/\text{sth10 1/sth11} \end{aligned}$$

7.13 Burst Expansion Ripple DAK

The Linear Regression equation for predicting Burst Expansion for Ripple DAK Bottle is as follows:

$$\begin{aligned} Y = & -0.1752 * \text{sth4} + -0.6241 * \text{sth6} + -0.0779 * \text{sth10} + -0.3355 * \text{sth11} + -0.1214 * \text{sth12} + - \\ & 0.1294 * \text{sth15} + 0.0458 * 1/\text{sth1} + 0.0770 * 1/\text{sth2} + 0.3213 * 1/\text{sth4} + 0.4465 * 1/\text{sth6} + 0.0091 \\ & * 1/\text{sth7} + 0.1480 * 1/\text{sth10} + 0.0282 * 1/\text{sth11} + 0.3127 * 1/\text{sth15} + 0.0351 * \text{sth1 sth14} + 0.0334 \\ & * \text{sth2}^2 + 0.0571 * \text{sth5 1/sth1} + -0.0315 * \text{sth8 1/sth8} + -0.0097 * \text{sth9 1/sth8} + -0.0080 * \text{sth9} \\ & 1/\text{sth10} + 0.0191 * \text{sth10 sth15} + 0.1225 * \text{sth11}^2 + -0.0016 * \text{sth11 1/sth7} + -0.0698 * \text{sth11} \\ & 1/\text{sth9} + -0.0247 * \text{sth12}^2 + -0.0126 * \text{sth12 1/sth5} + -0.0426 * \text{sth12 1/sth7} + -0.0467 * \text{sth13} \\ & 1/\text{sth13} + 0.1375 * \text{sth14 1/sth9} + 0.0709 * \text{sth15 1/sth6} + 0.1281 * 1/\text{sth6}^2 + 0.0190 * 1/\text{sth7} \\ & 1/\text{sth10} + 0.0204 * 1/\text{sth8}^2 + 0.0069 * 1/\text{sth8 1/sth9} + 0.0005 * 1/\text{sth9 1/sth10} + 0.0506 * \\ & 1/\text{sth13}^2 + 0.0708 * 1/\text{sth13 1/sth14} \end{aligned}$$

7.14 Empty Top Load 20.5 AXL

The Linear Regression equation for predicting Empty Top Load for 20.5g AXL Bottle is as follows:

$$\begin{aligned} Y = & 1.4602 * \text{sth4} + 1.1842 * \text{sth6} + 3.9567 * \text{sth7} + 6.9335 * \text{sth11} + 0.9921 * \text{sth12} + 4.8660 * \\ & \text{sth13} + -0.2423 * \text{sth1 sth2} + -1.1786 * \text{sth2 sth3} + 1.1381 * \text{sth2 sth15} + 3.8285 * \text{sth4 sth11} + \\ & 0.7463 * \text{sth4 sth15} + -1.4621 * \text{sth5 sth6} + -0.8441 * \text{sth6 sth7} + 0.2146 * \text{sth6 sth13} + 1.3813 * \\ & \text{sth7 sth11} + -0.3802 * \text{sth10 sth11} \end{aligned}$$