JCTA Journal of Computing Theories and Applications ISSN:3024-9104

Research Article

Strategic Feature Selection for Enhanced Scorch Prediction in Flexible Polyurethane Form Manufacturing

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Abstract: The occurrence of scorch during the production of flexible polyurethane is a significant issue that negatively impacts foam products' resilience and generally jeopardizes their integrity. The likelihood of foam product failure can be decreased by optimizing production variables based on machine learning algorithms used to predict the occurrence of scorch. Investigating technology is required because prevention is the best approach to dealing with this problem. Hence, machine learning algorithms were trained to predict the occurrence of scorch using the thermodynamic profile of polyurethane foam, which is made up of recorded production variables. A variety of heuristics algorithms were trained and assessed for how well they performed, namely XGBoost, Decision trees, Random Forest, K-nearest neighbors, Naive Bayes, Support Vector Machines, and Logistic Regression. The XGboost ensemble was found to perform best. It outperformed others with an accuracy of 98.3% (i.e., 0.983), followed by logistic regression, decision tree, random forest, K-nearest neighbors, and naïve Bayes, yielding a training accuracy of 88.1%, 66.7%, 84.2%, 87.5%, and 67.5% respectively. The XGBoost was finally used, yielding 2-distinct cases of non(occurrence) of scorch. Ensemble demonstrates that it is quite capable and is an effective way to predict the occurrence of scorch.

Keywords: Feature selection; Foam production; Machine learning; Polyurethane; Scorch; XGBoost.

Received: December, 4th 2023
Revised: February, 27th 2024
Accepted: February, 28th 2024
Published: February, 29th 2024

1. Introduction

Scorch is a menace in the production of polyurethane foam [1], and studies have used machine learning to create predictive ensembles to forecast the menace's existence. Polyurethane foam is a porous, cellular-structured synthetic created when diisocyanates and polyols mix together. Its structure consists of a mix of solids and gases [2]. Blowing agents create the gas, while solids are polyurethane elastomer. Comparing their substitute material, polyurethane foams are used everywhere in our environment due to their incredibly beneficial physical characteristics [3]. They are excellent for thermal and sound insulation, beds, auto interiors, furniture, encapsulating components, carpet underlays, and packaging, amongst other applications for their low density and thermal conductivity [4]–[6].

Levchik et al. [7] used water to replace chlorofluorocarbons, and it was found to increase the likelihood of scorch occurrence in flexible polyurethane, where fire retardants were also used as formulating ingredients. While not all fire retardants cause scorch [8] – interaction between fire retardants and aniline from -NH2 is always present in water-blown polyurethane foam. They believed this interaction cannot be disregarded in the crucial discussion of scorch occurrence in polyurethanes. Yu-Zhong et al. [3] concurred with the importance of this interaction in scorch occurrence. They proposed a revolutionary way to mitigate this – adding antioxidants to the formulation lessens the effects of fire retardants. Secondary antioxidants are extensively used in extreme conditions and low-density foam productions where the raw materials have high moisture contents or contain fire retardants as a production component. However, Nabata et al. [9] proposed heating foam samples in a microwave oven and observing its cure to estimate the likelihood of scorching and test various fire retardants for flexible polyurethane foam. Its drawback is that it requires a lot of time, energy, and resources and is very laborious in terms of sustainability compared to using a model that can simulate the same result in a shorter amount of time [10]. Also, changes to various suspected contributing factors are based on a trial-and-error basis, requiring several iterations and trials to achieve the desired result [11]. There is also the ineffectiveness due to waste of resources.

Scorch is visually recognized only after curing has taken place and the foam slab is split open to expose the core [12]. This means adjustments during production are not a smart decision as experts only make adjustments prior to scorch occurrence. Recently, Demassa [13] noted the merits of a scorch inhibitor that lessens it in foam discoloration. The method used morphological and chemical changes in the core of scorched flexible polyurethane foam. Its drawback is that scorch inhibitors are known to contribute to foam discoloration (not necessarily from scorch) brought on by exposure to sunlight and warehousing fumes [14]. The difficulty of generalizing these recommendations for all production processes is that they do not adequately take into account the various specifications of supplied polyurethane raw materials from various suppliers, particularly polyols, diisocyanates, and other conditions of the production plants (in the case where scorch is typically promoted as a result of mechanical defects) [15].

The ensemble technique seeks to combine many base learner models by fusing them into a single classifier [16], [17]. It achieved this feat using either (a) bagging (bootstrap aggregation) iteratively generates a training subset from the original dataset via aggregating the various results using the majority voting (for classification) or averaging (for regression), and (b) boosting sequentially merges or combines many weak learners into one powerful learner with enhanced accuracy. Each learner impacts its successor, considering the weakness and performance of the base models [18]–[20]. The focus of bagging and boosting is to achieve better prediction by mitigating bias, which assigns higher weights to misclassified outcomes and lesser weights to accurately predicted outcomes [21], [22]. We adopt the Xtreme Gradient Boost (XGBoost) and compare its results against known ensembles using a retrieved dataset to predict scorch formation and occurrence in foam manufacturing accurately.

Also, a major challenge to classifiers is the appropriate selection of features to predict their underlying distribution (in both classification and regression cases). Thus, besides selecting the right dataset for use by the learners/classifiers, the chosen heuristics also have to adequately and appropriately select the required parameters to avoid overparameterization of the heuristics, which can often mislead the classifier into poor generalization (i.e., overfitting and overtraining of the ensemble or model). To curb this, we also perform feature selection using the appropriate foam manufacturing dataset to help our ensemble curb the issues of poor generalization.

1.1. Foam Production: A Literature Review

Chlorofluorocarbons (CFCs) were previously used as the primary blowing agent in producing flexible polyurethane foams [23]. Its emission effect on the environment led to its ban, And it was substituted with water [9]. The reaction of water and isocyanate in polyurethane foam production is highly exothermic as it raises the foam temperature during manufacturing. Thus, industry experts are faced with finding the right proportion of these constituents to prevent the occurrence of scorch [24]. Scorch is the slight coloration during the produced foam slab. It reduces a foam's degree of compactness and decreases its durability. Foams with scorch quickly suppress [25], known causes include oxidation of phenols and amines, and non-polymeric components are responsible for the discoloration [26]. In addition, the high-exothermic reaction between isocyanate and water also causes temperature rise [27]. A scorch is a heat-induced change in polyurethane foam production from inadequate exposure that prevents proper dissipation so that the trapped heat in the fully formed foam causes a scorch at its cure phase [28], [29]. Some of the known impacts include (a) low resilience and elasticity, (b) porous cell structure and consequent low load-carrying capacity, (c) reduced life span, (d) generation of high-volume waste, (e) poor utility of feed resources, and (f) reduced profitability [30].

Conventional remedies to scorch include: (a) adding fire retardant when manufacturing polyurethane foam, (b) using antioxidants and organic acids such as salt as anti-scorch constituents [31], (c) removal of excess isocyanate in the formulation to yield faster reaction with water, (d) use of inhibitors like halogenated phosphate ester additives in proper ratio with diphenylamine derivative and hydroquinone. Even so, there is increased worry about emissions from these chemicals' environmental friendliness and the rise in operating costs they provide [32]. The available options for tackling scorch depend heavily on the need for highly skilled experts to properly navigate the proportioning of these additives into the system. A more effective and cost-efficient method would be to simulate the process and aim to respond to any case of scorch occurrence before carrying out the process physically.

1.2. Feature Selection (FS)

FS is a method to reduce dimensionality by removing irrelevant features or parameters [33], [34]. As a pre-processing step in machine learning tasks, FS has been successfully used in a variety of applications as its usefulness are numerous to include (and not limited to) overcoming the burden of parameter dimensionality and eliminating irrelevant cum docile features [35]–[37]; Thereby, leading to enhanced performance of the machine learning heuristics for both regression or classification task. FS becomes critical in domains where cost and the measure of attributes are of utmost importance. This is because it can safely streamline the collection of data vis-à-vis the required format to fasten a model's construction as well as assist in unraveling cum interpreting the innate structure of the dataset [38], [39].

FS is grouped into either (a) filter approach, which hinges on the inherent properties of data to select appropriate features devoid of classification learning [40], [41], and (b) wrapper approach, which uses a classifier to assess the qualities of the feature(s) [42]–[44]. The latter approach is computationally less cost-effective when compared to the filter approach – as the chosen features are often inclined toward the heuristics or classifier adopted/adapted [45], [46]. Assessing the goodness of fit of the FS is such that it targets its efficacy or efficiency within the host algorithm or heuristics. Evaluating the FS can be quite easy if the ground truth (i.e., real relevant feats) is known. However, this is not often so in real-world data, owing to the fact the ground truth for real-world data is not always available for training [47]–[50].

Each classifier that performs well on the training dataset may not blend well on the new test dataset and may overfit the model. Thus, in some cases – the k-fold cross-validation or its variant is engaged to separate training/test data. Data is divided into k equal-sized folds – so that for each k-iterations, 1-fold is reserved for testing while the remainder $k-1$ folds are used in training. Thus, FS is executed before dimensionality reduction is achieved.

2. Material and Method

2.1. Data Gathering

The dataset used was collected from Winco Foam Limited, Benin City. The dataset consists of 15-features namely: polyurethane throughput, calcium throughput, TDI throughput, water throughput, polyurethane dials-set, calcium dial-set, TDI dial-set, water dial-set, quantity of polyurethane, quantity of calcium, quantity of TDI, quantity of water, polyurethane water content, production time, and scorch – all of which sums up to about 8,540 data-points as in table 1. These are associated with the formation of a scorch on the retrieved dataset spreadsheet (from its unstructured format) [51]–[54].

2.2. Proposed Machine Learning Framework

We adopt the extreme boosting algorithm with the following steps:

1. **Step 1 – Data Collection and Cleaning**: With data recorded during production – we used the Google Play Scraper Library for Python to extract as in [55]. It is then cleaned to yield the optimized form via pre-processing and cleaning actions to yield a restructured dataset with the description in Table 1 [56]–[58].

Table 1. Dataset Description

Items	Poly thru	Calc thru	TDI thru	Water thru	Poly dial	Calc dial	TDI dial	Water dial	Qnty Poly	Qnty Calc	Qnty TDI	Qnty Water	Prod Time	Scorch
Count	36.000	36.000	36.000	36.000	36.000	36.000	36.000	36.000	36.000	72.000	72.000	72.000	0.7.200	72.000
Mean	71.996	13.142	54.643	4.4988	13.469	18.280	68.111	278.28	1485.5	293.86	1141.5	96.276	0.0800	20.908
Std	9.3113	1.9250	1.4917	0.0865	3.6109	2.1598	0.8544	10.053	729.86	175.89	573.91	46.816	0.0004	10.501
Min	45.000	10.000	50.250	4.3500	6.6000	15.000	67.000	270.00	291.00	43.650	213.40	17.190	0.0008	3.8800
25%	75.000	11.250	54.903	4.4010	11.300	16.100	68.000	270.00	1042.4	194.06	756.23	65.965	0.0008	14.690
50%	75.000	14.005	55.420	4.5600	14.050	18.800	68.000	280.00	1350.0	262.02	1042.5	89.645	0.0008	20.002
75%	75.000	15.000	55.462	4.5640	14.950	20.500	68.000	280.00	1989.0	383.43	1470.3	125.25	0.0008	28.193
Max	80.000	16.000	55.610	4.7000	23.610	20.800	71.000	318.00	3000.0	923.85	2625.0	228.40	0.0008	50.000

2. **Step 2 – Machine Learning Heuristics**: We used eXtreme Gradient Boosting to help us classify data points effectively. The Extreme Boosting (XGBoost) is a decision tree ensemble that leverages a scalable Gradient Boost model [59]. It becomes quite efficacious and stronger as it combines weak learners over a series of iterations to find an optimal fit solution. We achieved this via an additional expansion of its objective function by minimizing the loss function to create the variant used to control the trees' complexity. XGBoost yields a better optimal fit by combining the predictive power of many weak learners (that contribute knowledge about the task) to the ensemble [19], thus yielding a collection of stronger learners. As in this study, for each candidate to be trained x_i and its corresponding labels y_i – we predict using XGBoost as in Equation (1).

$$\hat{Y}_i^t = \sum_{k=1}^{t} f_k(x_i) = \hat{Y}_i^t + f_k(x_i) \tag{1}$$

To yield a better outcome, we expand the objective function via a loss function $l(Y_i^t, \hat{Y}_i^t)$ and its regularization term $\Omega(f_t)$). This ensures that overtraining does not occur, ensures the training data are fitted well, and re-calibrates the solution to ensure they are within the upper and lower bounds of the solution. The regularization term ensures the tree complexity is appropriately fit. We tune the loss function for higher accuracy and tune the regularization terms to help the ensemble avoid parameter overfitting, as in Equation (2).

$$L^t = \sum_{i=1}^{n} l\left(Y_i^t, \hat{Y}_i^{t-1} + f_k(x_i)\right) + \Omega(f_t) \tag{2}$$

3. **Step 3 – Feature Selection with Chi-squared:** FS has a subset of features selected based on their relationship to the target variable. The filter approach measures the relevance of features with the output via a statistical test [60]. For this study, we use the chi-squared, which tests whether the occurrence of a specific feature and a specific class (existence of scorch) – are independent using their frequency distribution. Thus, in extracting features, the chi-squared extracts those features (as parameters) highly dependent on the output. We used the Python sklearn with mutual information 0 (i.e., no mutual information) and 1 (perfect correlation) between the features and the target variable (scorch). We rank all the features using the chi-squared test based on their association with the target variable. The threshold value is given by the Equation (3).

$$X = \frac{\sum x_i}{n} \tag{3}$$

The original dataset consists of 13 features that seek to categorize the correlation of the variables to class 1 (i.e., scorch). With the computed threshold value of 13.0231, a total of seven (7) features were selected from the original dataset thus: (a) polyurethane throughput, (b) calcium throughput, (c) water throughput, (d) quantity of water, (e) production time, (f) quantity of polyurethane, and (g) TDI dial.

4. **Step 4 - Hyper-Parameter Tuning** controls how much of the tree complexity and its corresponding nodal weights need to be adjusted in place of gradient loss. The lower the value, the slower we travel on a downward slope. It also ensures how quickly a tree abandons old beliefs for new ones during the training. Thus, as a tree learns, it quickly differentiates between important feats and others. A higher learning rate implies that the tree can change, learn newer features, and adapt flexibly and more easily. The ensemble uses the regularization term to ensure the model changes quickly, only to values that are within the lower and upper bounds. The ensemble does this to adjust its learning rate to avoid over-fitting and overtraining adequately. Hyper-parameters tuned include max_depth, learning_rate, and n_estimator. For best performance, the XGBoost ensemble must carefully tune these parameters.
5. **Step 5 – Retraining** is an applied ML scheme that estimates the learned skills of a heuristic technique on unseen data. It also seeks to evaluate model's performance about its accuracy and how well it has learned the underlying feats of interest via the resampling technique. To retrain – modelers choose several data folds (partitions) to ensure the

model is devoid of overfitting. We use stratified k-fold (rearranging the data to ensure that each fold is a good representation of the entire dataset) as in Algorithm 1 [61]–[64].

Algorithm 1. Stratified $\boldsymbol{k}$-fold cross-validation

```
INPUT: dataset
OUTPUT: k
shuffle the dataset
split/partition training dataset into k-number of folds
for k-number of iterations
    rearrange data into partitions: return k-fold = true
evaluate model: end
```

3. Results and Discussion

3.1. Training Evaluation and Hyper-Parameters Tuning

First, we tune the hyper-parameters using the tree's n_estimators, learning_rate, and max_depth, respectively. Table 1 lists the tuned hyperparameter (s) in training. We use the trial-n-error method to tune the hyperparameters and find the weight that yields the optimal solution. This improves the ensemble's fitness and deprives it of poor generalization. We observe the best-fit values as a learning_rate of 0.2, n_estimators of 500, and a max_depth of 6, respectively – during the training phase. This agrees with [65]–[67].

Table 2. Hyperparameter Configuration.

Hyperparameter	Definition	Trial and error	Best Value
N_Estimators	Number of trees in the ensemble	[100, 200, 300, 500, 700, 800]	500
Learning Rate	Step-size for learning	[0.05, 0.1, 0.2, 0.3, 0.5, 0.75]	0.2
Max-Depths	Max. number of trees depth	[1, 2, 4, 5, 6, 8, 10]	6

To compute the accuracy of the ensemble – we evaluate its performance using Equation (4) – yielding Figure 1 as the confusion matrix as supported by [68]–[70].

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN} \tag{4}$$

Prediction	Actual	
	507	**19**
	2	**523**

Figure 1. Confusion Matrix

The performance of the various ensembles is in Table 3. The XGBoost yields an accuracy of 98.3% (i.e., 0.983). The benchmark heuristics used to measure how well our XGBoost performed resulted in the following prediction accuracies as logistic regression 0.881 (i.e., 88.1%), decision tree 0.667 (i.e., 66.7%), random forest 0.842 (i.e., 84.2%), k-nearest neighbor 0.875 (i.e., 87.5%), support vector machine 0.679 (i.e., 67.9%) and naïve bayes 0.661 (i.e., 66.1%) respectively. These results are based on the adapted dataset used in Table 1.

We have successfully implemented a variety of algorithms with k-fold cross-validations and resulting predictions on the occurrence and presence of scorch in the production of flexible polyurethane foam. The XGBoost ensemble outperformed other algorithms for the given dataset with an accuracy of 98.3% [71]. The ensemble yielded 2-distinct predictions for the occurrence of scorch with k-fold re-training as in Table 4.

Table 3. Performance metrics of 'before' and 'after' Feature Selection and Comparison

Method	Before Feature Selection				After Feature Selection			
	Accuracy	Precision	Recall	F1	Accuracy	Precision	Recall	F1
Logistic regression	0.881	0.832	0.840	0.849	0.899	0.881	0.853	0.881
Decision tree	0.713	0.653	0.653	0.645	0.732	0.657	0.637	0.667
Random forest	0.882	0.704	0.771	0.812	0.885	0.842	0.822	0.842
K-nearest neighbor	0.771	0.743	0.765	0.832	0.773	0.712	0.715	0.875
Support vector machine	0.667	0.639	0.614	0.651	0.692	0.673	0.543	0.679
Naïve Bayes	0.534	0.553	0.562	0.649	0.671	0.567	0.562	0.661
XGBoost	0.955	0.959	0.932	0.951	0.988	0.978	0.932	0.983

Table 4. Predicted Values with the value '1' indicates the presence of scorch

Poly thru	Calc thru	TDI thru	Water thru	Poly dial	Calc dial	TDI dial	Water dial	Qnty Poly	Qnty Calc	Qnty TDI	Qnty Water	Prod Time	Scorch
75	11.25	55.42	4.564	11.3	75	68	280	478.5	71.77	101.1	353.58	6.38	1(Yes)
75	11.25	55.50	4.564	11.3	75	68	280	1500	225	91.28	1110	20	0(No)

Data access was severely constrained as facilities yield large amounts of production data daily. Its documentation is rather antiquated and is quickly lost when not properly used. The dataset used was manually collected and restricted to only a short duration [72].

Furthermore, the plot of Figure 2 shows a relative scorch occurrence in the production data even when all pointer outliers indicate 'no scorch occurrence' and agree with [73]–[75]. It is worth noting that the study seeks to predict if the mix of all variables to a certain degree can significantly cut down the scorch occurrence bin.

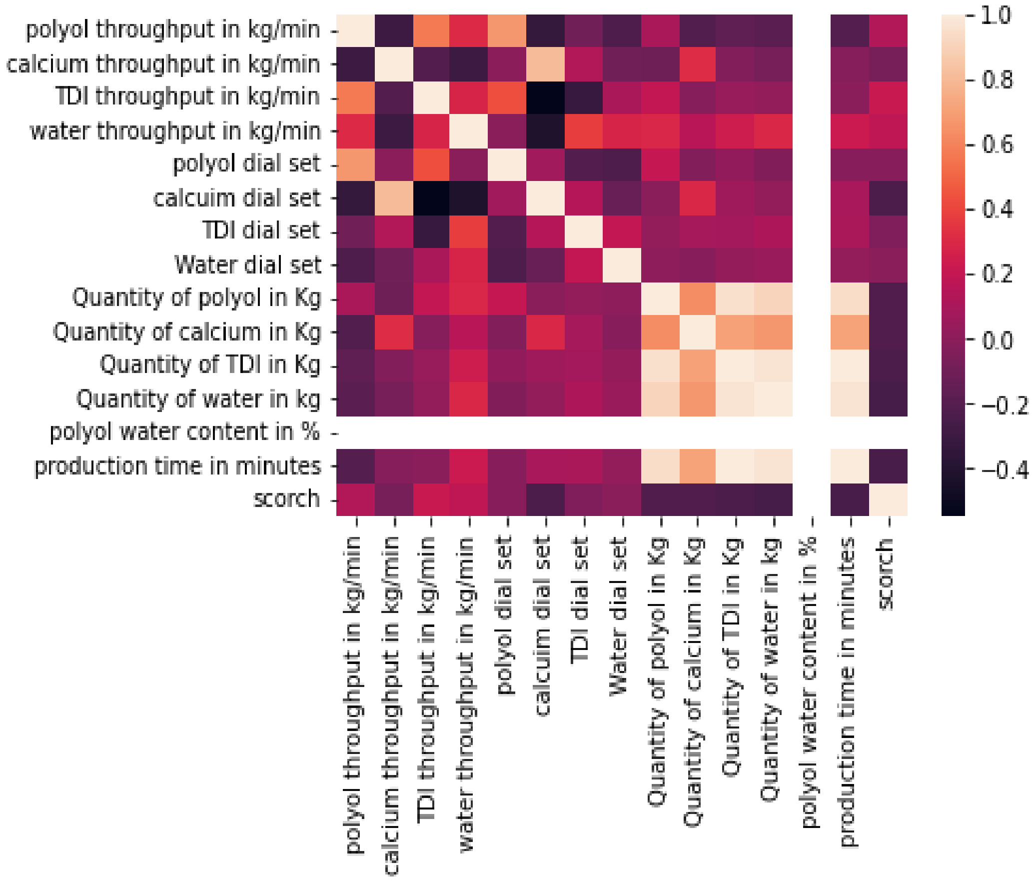

Figure 2. The heatmap of all variables against each other

The distribution plot, as in Figure 3, helps to ascertain the skewness of the most important column head 'scorch' in reference to density. Its data is fairly distributed across the upper quartiles from the mean. Thus, minimizing the outlier effects as agreed by [76]–[80].

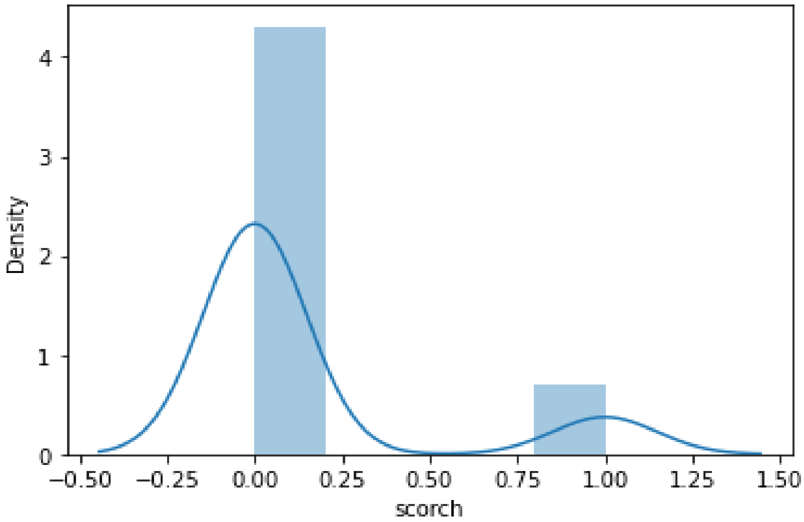

Figure 3. Data Distribution plot

3.2. Discussion of Findings

The scatter plot in Figure 4 supports the prediction that an excessive amount of water conducts too much heat; And in turn – raises the temperature profile of the flexible polyurethane foam slab's core. This, in turn, also increases the likelihood that scorch formation will occur in flexible foam production.

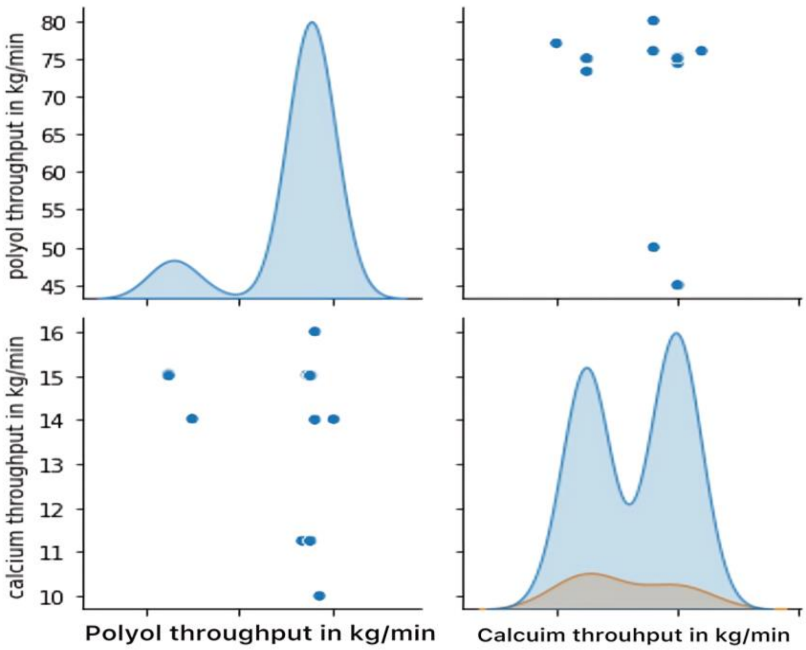

Figure 4. The scatterplot of polyurethane without water versus calcium throughput

Figure 5 supports the addition of excess water, showing a high correlation between temperature and time in the foam slab during the flexible foam production. This implies that the likelihood of scorch occurring is a function of time, water, and calcium in the foam slab.

The addition of water as a universal solvent – has consequently yielded a connection and correlation between water and scorch [81]–[83] – which is already known feat. It further suggests that water is in the heat map, unveiling a variety of intertwined relationships between other features, the polyurethane and water in the dataset [84]–[86]. All negative values on the correlation also yield a corresponding negative relationship between both variables and vice versa. And this can be visually confirmed from the pair plots as supported by [87]–[89].

Meanwhile, NaN (not a number) indicates no relationship at all. The reason behind this is that the value of the column 'polyol water content in %' is constant throughout. To prevent overfitting in our model, this column is flattened or brought down before deploying our machine-learning algorithm, which agrees with [90]–[92]. These correlation numbers are illogical at first glance. But this is where using the machine learning algorithm is advantageous. These algorithms trace the entangled connections, interpret how each variable interacts with the others, and influence the column (variable) that we want to predict [93]–[95].

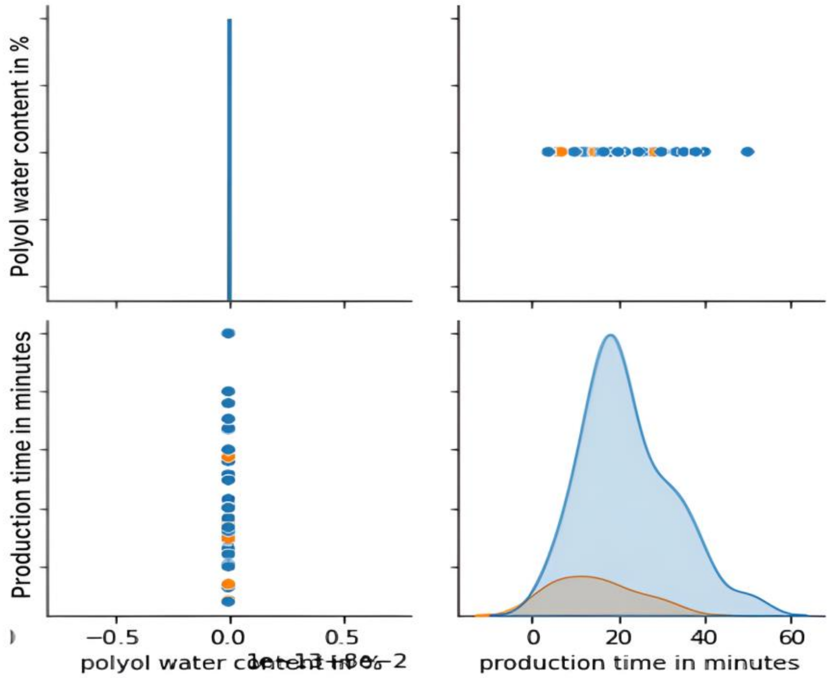

Figure 5. Scatterplot of production time with polyurethane, calcium and water

4. Conclusions

With the current surge in technological development and the widespread adoption of new technology-driven business strategies, businesses can operate more efficiently, productively, and profitably. Despite the enormous amount of data generated daily, we have observed that the polyurethane industry has lagged behind in developing cutting-edge data analytics and data science technologies. So, for the future of this industry, this study is a positive step and should be improved upon.

Author Contributions: Conceptualization: F. Omoruwou, A.A. Ojugo and S.E Ilodigwe; Methodology: F. Omoruwou, A.A. Ojugo, S.E. Ilodigwe; Software: S.E Ilodigwe and A.A. Ojugo; Validation: A.A. Ojugo and F.Omoruwou; Formal Analysis: S.E Ilodigwe; Investigation: F.Omoruwou, A.A. Ojugo and S.E Ilodigwe; Resource: F. Omoruwou and S.E Ilodigwe; Data Curation: A.A. Ojugo and S.E Ilodigwe; Writing—original draft preparation: F. Omoruwou and S.E Ilodigwe; Writing—review and editing: F. Omoruwou and A.A. Ojugo; Visualization: A.A. Ojugo; Supervision: F. Omoruwou; Project administration: F. Omoruwou and A.A. Ojugo; funding acquisition: All.

Funding: This research received no external funding.

Acknowledgments: Winco Form Production Company, Benin-City, Edo State

Conflicts of Interest: The authors declare no conflict of interest.

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