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Monitoring the oxidative deterioration process in modified atmosphere packaged ground meat using a machine learning-based model

Modifiye atmosfer paketli kıymada oksidatif bozulma sürecinin makine öğrenmesi tabanlı model ile izlenmesi

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Abstract

This study investigated the use of a machine learning approach to predict oxidative changes during the storage of modified atmosphere packed (MAP) ground beef. Peroxide, TBARS, titratable acidity, and mercaptan levels were used as indicators for oxidative deterioration and integrated into Random Forest model. The obtained model had an R^2 value of 0.867, indicating acceptable prediction performance with low prediction errors. The model achieved a classification accuracy of 0.914. Furthermore, it was determined that the peroxide value is the most effective parameter reflecting the early stage of lipid oxidation, while the TBARS value represents the gradually developing secondary oxidation process. The results suggested that evaluating oxidative indicators using machine learning can be a reliable tool for monitoring freshness of MAP-packed ground beef.

Keywords: Oxidative deterioration, Machine learning, ground beef, Modified atmosphere packaging.

Öz

Bu çalışma ile modifiye atmosfer paketli (MAP) kıymanın depolanması sırasında oksidatif değişiklerin tahmin edilmesi için makine öğrenmesi yaklaşımının kullanımı araştırılmıştır. Peroksit, TBARS, titrasyon asitliği ve merkaptan seviyeleri oksidatif bozulma göstergeleri olarak kullanılmış ve rastgele orman modeline entegre edilmiştir. Elde edilen modelin R^2 değeri 0.867 olarak belirlenmiş ve düşük tahmin hataları ile kabul edilebilir bir tahmin performansı göstermiştir. Model 0.914'lük bir sınıflandırma doğruluğu elde edilmiştir. Ayrıca, peroksit değerinin lipid oksidasyonunun erken sürecini yansıtan en etkili parametre olduğu, TBARS değerinin ise kademeli olarak gelişen ikincil oksidasyon sürecini temsil ettiği belirlenmiştir. Sonuçlar, makine öğrenmesi kullanılarak oksidatif göstergelerin değerlendirilmesinin, MAP ambalajında paketlenmiş kıymanın tazeliğini izlemek için güvenilir bir araç olabileceğini göstermiştir.

Anahtar kelimeler: Oksidatif bozulma, Makine öğrenmesi, Sığır kıyması, Modifiye atmosfer paketleme

1 Introduction

Chemical and biochemical changes that occur during the storage of meat and meat products are important factors that directly affect product quality and shelf life. These changes arise from complex interactions between enzymatic activity, microbial growth, and physicochemical reactions, which affect sensory properties, nutritional value, and product safety. Among these degradation pathways, lipid oxidation is considered as one of the most critical mechanisms responsible for quality deterioration in meat systems [1].

Lipid oxidation, also referred to as "autooxidation," is a process that occurs as a result of radical chain reactions consisting of initiation, propagation, and termination phases. During these reactions, unsaturated fatty acids are oxidized and formed primary products such as conjugated dienes and hydroperoxides, while secondary oxidation products such as aldehydes are formed in later stages. These compounds can interact with proteins, leading to changes in the flavor, odor, color stability and nutritional quality of meat products [2-4]. Furthermore, it can also trigger protein oxidation, reducing functional properties such as protein solubility and water-holding capacity. [1, 5, 6]. Therefore, oxidative deterioration should be considered a dynamic, multidimensional and time-dependent process involving changes in multiple quality parameters. However, evaluating oxidative deterioration by considering together multiple quality parameters and modeling the relationships between these parameters is quite complex [4, 7]. Traditional approaches often focus on evaluating the effects of parameters individually, which may be insufficient to comprehensively explain the dynamic and multifaceted nature of oxidative degradation.

In recent years, machine learning (ML) methods have been increasingly applied in food quality assessment due to their potential to examine, model and predict relationships among multiple variables [8, 9]. ML approaches evaluate multiple quality parameters simultaneously. This makes it possible to understand and interpret nonlinear relationships that are difficult with traditional statistical methods. However, current studies primarily focus on predictive performance rather than identification of oxidative deterioration stages or integrating oxidation-related parameters into a unified quality index [10-12]. Furthermore, there is a need for approaches that not only predict quality

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changes but also provide information on the progression of the oxidative degradation process.

The Random Forest algorithm is widely used in data mining due to its high accuracy and ability to work efficiently with large datasets. It also stands out because of its capacity to evaluate numerous variables simultaneously and its ability to determine the significance of those variables [13, 14]. This algorithm has yielded successful results in meat products [15, 16]. Therefore, it is hypothesized that this algorithm can also be effective in MAP-packed products, which are widely preferred in retail due to their ability to slow down oxidative reactions and extend shelf life [17]. In addition, TBARS and peroxide levels, which are used as primary chemical indicators in the evaluation of oxidative degradation [18, 19], are also frequently used in algorithms [20-22].

This study aims to evaluate oxidative changes occurring during the storage of modified atmosphere packed ground beef samples using an ML model. For this purpose, it is hypothesized that integrating multiple oxidative indicators into a combined ML framework will allow for more accurate determination of the oxidative deterioration stages affecting meat quality during storage. A model was developed using the Random Forest algorithm that combines the overall quality of the product under a single quality index, using TBARS, peroxide, titratable acidity, and mercaptan values determined during the storage of modified atmosphere packed ground beef samples.

2 Material and methods

2.1 *Storage of MAP-packaged ground beef*

In this study, MAP packed ground beef samples were obtained from a local producer. Modified atmosphere conditions consist of a mixture of 30% oxygen (O_2), 20% nitrogen (N_2), and 50% carbon dioxide (CO_2). Samples were transported under cold chain conditions in the laboratory and stored at +4 °C for specified shelf life by the manufacturer (15 days). During the storage period, samples were taken at 4h intervals to determine the oxidative changes and analyses were performed to determine TBARS, peroxide, titratable acidity, and mercaptan levels. A total of 900 analysis data points were obtained from 180 minced meat samples, through repeated measurements taken at 4-hour intervals during a 15-day storage period; 9 outlier observations were removed from the dataset using the Isolation Forest algorithm during the data preprocessing phase, and the remaining data were used in the model development process.

2.2 *Laboratory analysis*

2.2.1 *TBARS analysis*

Oxidative stability of MAP-packaged ground beef samples were determined by thiobarbituric acid reactive substances (TBARS) analysis [23]. Briefly, ground beef samples were homogenized by adding trichloroacetic acid (TCA) solution. The homogenates were filtered through Whatman No:1 filter paper and filtrates were mixed with thiobarbituric acid (TBA) solution and incubated (100°C for 40 min). Samples were cooled to room temperature and centrifuged. The absorbance was measured at 532 nm. Results were expressed as μmol MDA/kg sample.

2.2.2 *Peroxide Value*

The peroxide values of ground beef samples during storage were determined according to the [24]AOAC method. The samples were dissolved in acetic acid and chloroform mixture, followed by the addition of saturated potassium iodide solution. After samples were incubated in the dark, distilled water was added and titrated with sodium thiosulfate in the presence of starch indicator. Peroxide values were determined using the following Formula (1):

$$\text{Peroxide value} = \frac{\mathrm{V} \times \mathrm{N} \times 1000}{\mathrm{m}} \tag{1}$$

where V is the volume (ml) of sodium thiosulfate and m is the mass (g) of sample. Results were presented as meq O_2/kg sample.

2.2.3 *Titratable acidity analysis*

For Titratable Acidity analysis, samples were homogenized with distilled water and supernatants were taken. Then, supernatants were filtered with Whatman No:1 and titrated with sodium hydroxide solution in the presence of indicator [25]. Titratable acidity was determined using the following Formula (2):

$$\text{Titratable acidity (\%)} = \frac{\mathrm{V} \times \mathrm{N} \times 90}{\mathrm{m}} \tag{2}$$

where V is the volume (ml) of sodium hydroxide solution, N is the normality of sodium hydroxide solution and m is the mass (g) of sample. The results were expressed as lactic acid (%).

2.2.4 *Mercaptan content analysis*

Mercaptan contents of sulfur containing compounds in meat products were determined according to [26]Li, Li . Beef samples were homogenized with distilled water. The homogenates were washed with distilled water, filtered, and then stirred. Resulting filtrates were mixed with acetic acid and starch solution. The mixtures were titrated with iodine standard solution until a light blue color was obtained. Mercaptan content was determined using the following Formula (3):

$$\text{Mercaptan (mg/ 100 g)} = (((V - V_0) \times N \times 17)/m \times \frac{10}{100}) \times 10 \tag{3}$$

where V is the volume (ml) of iodine solution for sample, V_0 is the volume (ml) of iodine solution for the blank (mL), N is the molar concentration (mol/L) of standard iodine solution, m is the sample weight (g), 17 represent the milligrams of H_2S in 1 mL iodine standard solution. The results were expressed as mg mercaptan per 100 gram of sample.

2.2.5 *Statistical analysis*

All statistical analyses and ML procedures were performed using the Python (3.13.9). A regression model based on the Random Forest algorithm was developed. The Random Forest regression model was constructed using the scikit-learn library with 500 trees (n_estimators=500), random_state was fixed at 42 for reproducibility, and all processor cores (n_jobs=-1) were used to speed up the computation process. TBARS, peroxide, Titratable acidity and mercaptan values along with their derivatives (delta), were used as input variables. The dataset was normalized to a 0–1 scale using Min–Max (Formula (4)) normalization to ensure comparability among variables with different units and magnitudes.

$$X_{norm} = \frac{(X - X_{\min})}{(X_{max} - X_{min})} \tag{4}$$

Outliers were detected and removed from the dataset using the Isolation Forest algorithm. The dataset was divided into training and testing (80:20). Model performance was evaluated using coefficient of determination (R^2), mean absolute error (MAE) and root mean square error (RMSE) metrics. Additionally, quality index values categorized, and classification performance was analyzed using accuracy, precision, recall, and F1-score measures.

3 Results and discussions

Model prediction and performance parameters indicated that the obtained model had strong predictive capacity. The relationship between experimental data and model predictions generally followed a similar trend (Figure 1). However, moderate deviations between predicted and experimental values observed particularly at early and late storage stages. This may related to the low data density during the initial and final phases of the storage period.

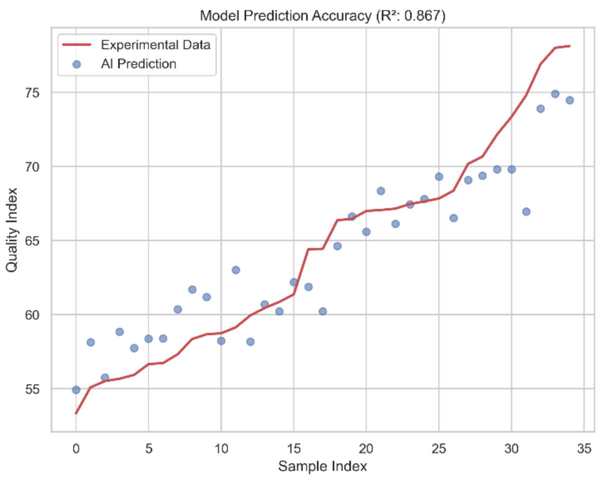

Figure 1. Model prediction accuracy

The coefficient of determination ($R^2 = 0.867$) shows that approximately 86.7% of the variance in the quality index is explained by the developed Random Forest model (Table 1). This coefficient value is considered high explanatory power in regression-based quality prediction studies [27, 28]. On the other hand, the combination of regression and classification criteria also indicated that the overall performance of the developed model is at an acceptable level. RMSE and MAE values were determined to be 2.5571 and 2.0477, respectively. These values indicated that the deviation between model predictions and actual values is low, and the overall prediction accuracy of the model is acceptable [28, 29]. This shows that the model can reliably determine changes in meat quality during storage. Specifically, it demonstrated that the model could be used as a reliable decision support mechanism in managing the shelf life of MAP-packed ground beef and determining critical freshness thresholds.

Table 1. Performance metrics of the Regression model

Metric	Value
R^2	0.867
RMSE	2.557
MAE	2.048

Results indicated that TBARS and peroxide values had non-linear relationship with model output (Figure 2). The peroxide values showed dramatic changes after a certain levels, whereas the TBARS values showed linear trend during storage. These results can be associated with lipid oxidation mechanisms and suggest that stages of oxidative degradation affect product quality and progresses at varying rates during the storage. Peroxides are formed during the early stage of oxidation and then, TBARS values representing secondary compounds and produced from the breakdown of these initial products [30, 31]. Overall, the model yielded results consistent with the biochemical process of lipid oxidation, and model predictions indicated that the expected oxidation pathways were followed.

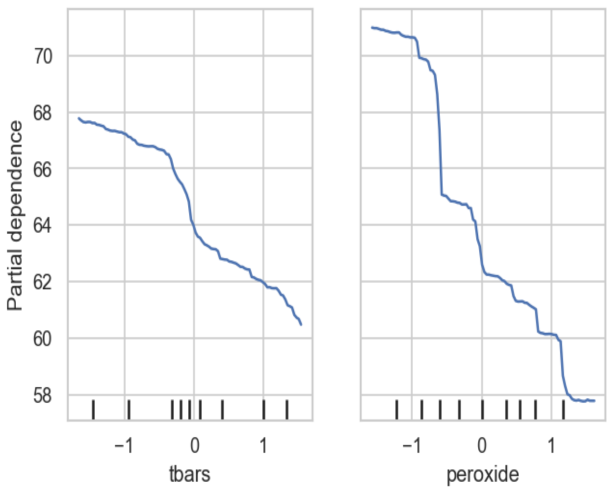

Figure 2. Marginal effects of oxidation parameters

The results showed that TBARS and peroxide values had a negative correlation with the quality index. Therefore, an increment in TBARS and peroxide values lead to a decrease in the predicted quality index. The marginal effects for peroxide had dramatic changes compared to TBARS. These results indicated that the model is more sensitive to peroxide induced changes and exceeding certain levels leads to more rapid and critical deterioration in quality [32]. In contrast, TBARS values had a smoother and more gradual trend and so more stable effect. This result is consistent with TBARS being secondary lipid oxidation products that forms in the later stages of oxidative degradation and typically increases continuously.

The time dependent oxidative quality changes for MAP packed ground beef defined the changes in meat quality throughout storage (Figure 3). The quality index ranged between 80 and 60 units during the storage period of approximately 350 hours (≈14.5 days). The strong alignment with the random forest model prediction curve (orange line) and the experimental data (blue line) suggested that the model reliably represents ground beef freshness (Figure 3) [33]. The oxidative degradation process can be divided into three main stages based on the prediction curve showing quality changes: a freshness phase (0–150 h), followed by a transition phase (150–250 h), and a late oxidation phase (>250 h). These determined stages are similar and consistent with the kinetics of lipid oxidation in meat systems. Changes in some factors such as reaction rate and substrate availability can affects initiation, propagation, and termination phases [34].

In Figure 3, the critical threshold value where the quality index falls under 45 units is shown with a red band. The quality index of the ground beef samples remained higher the threshold value throughout storage. However, it was determined that the freshness of the product started to decline after 250 hours of storage. This result showed that the quality index is driven by oxidative and biochemical reactions and progresses to a slow but irreversible stage [35].

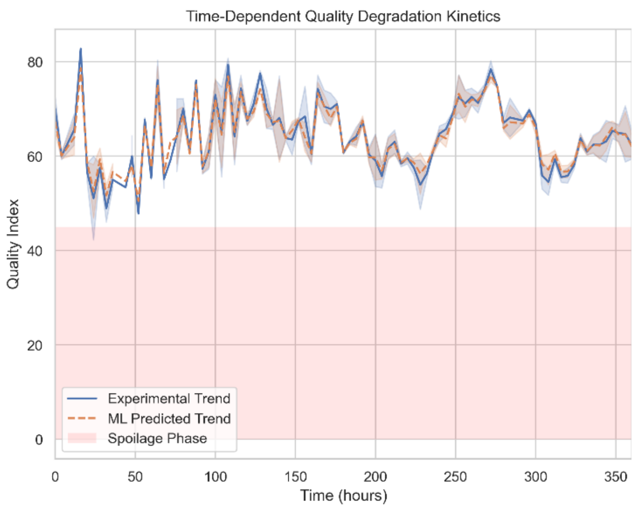

Figure 3. Dynamics of meat quality deterioration over time

The results indicated that peroxide values were the most effective parameter in monitoring of meat quality (Figure 4). Peroxide values explained approximately 43% of the relative significance in the prediction. The TBARS had a relative importance of approximately 20% and it indicated the importance of evaluating both primary and secondary oxidation products for accurate quality prediction. In addition, mercaptan and titration acidity also contributed significantly to the model prediction.

These results suggested that both dramatic and gradual reductions in the quality index were strongly associated with increases in peroxide levels. This has shown that the model primarily predicts of beef degradation based on primary lipid oxidation. On the other hand, the level of mercaptan contribution has shown that the deterioration of ground beef is affected by lipid oxidation as well as protein degradation. The results indicated that changes in meat quality during storage are due to simultaneous lipid and protein degradation processes rather than a single degradation pathway. Furthermore, the relatively low significance of parameters such as acidity_delta and mercaptan_delta, which shows variations between consecutive measurements, indicated that the model is less affect by temporal variation. Consequently, peroxide and TBARS values were primary indicators of meat quality and the mercaptan values provided complementary information.

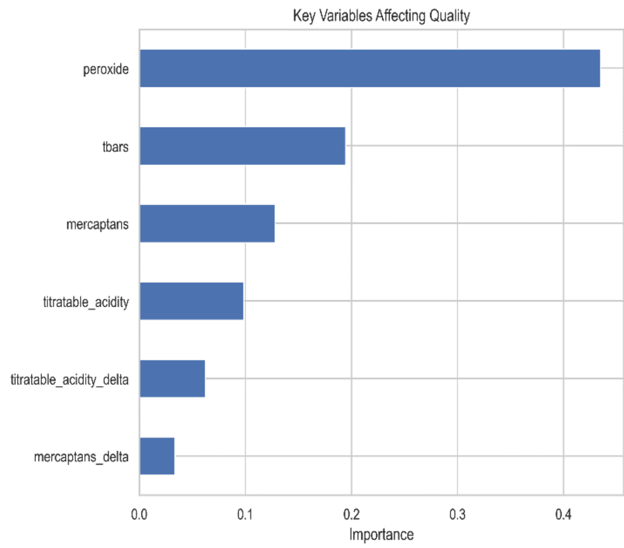

Figure 4. The importance levels of parameters in predicting meat quality

The regression model predicts the overall quality index of the meat product as a continuous value. In shelf-life management and decision support systems, quality levels must be expressed categorically. Accordingly, the predicted quality index scores in present study were classified into three distinct categories based on predefined thresholds: fresh, acceptable, and spoiled. Samples with a quality index above 75 are considered fresh, values between 60 and 75 are acceptable, and values below 45 are defined as spoiled.

The accuracy value for the model's classification performance was determined as 0.914 (Table 2). This showed that the model could correctly classify 91% of the samples. Moreover, the F1-score was 0.874 and this indicates that the model exhibited balanced performance across classes and particularly sensitive to class balance. In addition, the precision per class and recall of model were determined as 0.836 and 0.914, respectively. These values demonstrated that the model exhibits consistent performance both numerical predictions and practical quality classification tasks.

Table 2. Model Classification Performance

Metric	Value
Accuracy	0.914
F1-score	0.873
Precision	0.836
Recall	0.914

The confusion matrix shows distinguishing performance in quality categories of the developed model (Figure 5) [36]. The highest success rate of the model for classification was determined in acceptable quality category. The fact that all samples belonging to acceptable category were correctly predicted indicates that the model can reliably identify the stage at which oxidative reactions have begun but have not yet reached a critical degradation level. In addition, many samples classified as Fresh were predicted as Acceptable. This can related with an overlap between classes because quality parameters showed limited differences in the early stages of storage. Chemical changes were still minimal in the initial stage of lipid oxidation, which makes it difficult for the model to distinguish classified as Fresh products from classified as Acceptable products. This is consistent with the spoilage process of meat is generally a gradual process rather than a sudden one. In contrast, the Spoiled category was predicted with full accuracy, which shows that the model reliably distinguishes products approaching their expiration date or reaching critical spoilage levels [31]. The fact that many ground beef samples remained unspoiled until their expiration date demonstrates that the predictions of model are both realistic and reliable [37].

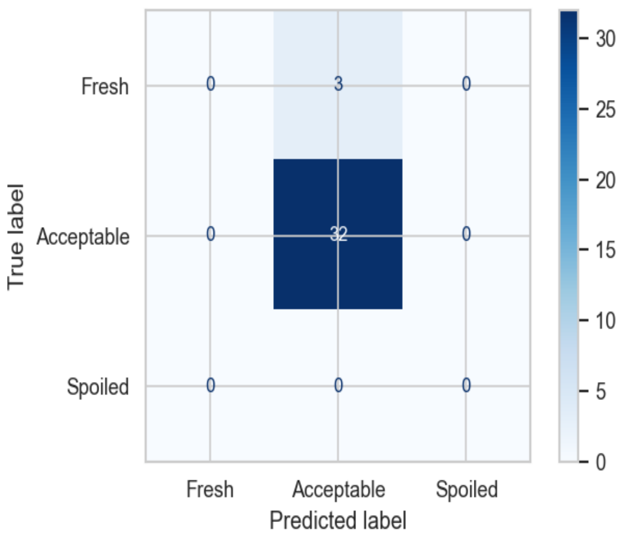

Figure 5. Confusion matrix for quality category classification

4 Conclusion

The results of present study showed that multiple oxidative indicators including peroxide, TBARS, acidity, and mercaptan could be integrated into a single Random Forest model. The peroxide values were the most critical parameter for the developed model and model predicted meat quality with high accuracy. Three distinct oxidative stages were classified by the developed model: the initial freshness stage (0–150 hours), the accelerated oxidative reaction stage (150–250 hours), and the advanced oxidation stage (>250 hours). The fact that many samples remained acceptable until their expiration date suggested that the model could help optimize shelf-life management and potentially predicting the expiration date.

The developed model provides a more comprehensive assessment of oxidative deterioration in MAP packed ground beef compared to traditional methods. Furthermore, the model offers both a scientific and practical tool for meat quality management by combining multiple parameters into a single quality index.

Conflict of interest

The authors declare that have no conflicts of interest related to this article.

Similarity rate (iThenticate): 9%

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