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Integrating physicochemical analysis and artificial intelligence prediction to monitor degradation of edible oils during repeated frying and storage

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Summary

This study evaluated physicochemical changes in edible oils during repeated frying and storage using a hybrid analytical framework integrating experimental analysis with artificial intelligence (AI)-based predictive modelling. Eleven edible oils were analysed for peroxide value, iodine value, acid value, free fatty acids, viscosity, refractive index, moisture content, and specific gravity using standard methods. Repeated frying significantly increased peroxide value, acid value, free fatty acids, and viscosity, indicating oxidative and hydrolytic degradation, while iodine value decreased due to thermal oxidation of unsaturated fatty acids. Storage conditions affected oil stability; oils in transparent plastic bottles under light showed greater oxidative deterioration than those in dark glass containers. To predict oil degradation, random forest regression was benchmarked against multiple linear regression, support vector regression, and gradient boosting. Random forest achieved the best predictive performance (coefficient of determination $R^2 = 0.92$, root mean square error $RMSE = 0.52$), with peroxide value combined with frying cycle number (34 %), acid value with free fatty acids (26 %), and viscosity with specific gravity (18 %) as primary predictor groups. These findings demonstrate the practical utility of AI-assisted predictive monitoring for rapid edible oil quality assessment.

Keywords

physicochemical properties; peroxide value; frying stability; edible oils; artificial intelligence; random forest model

Cooking oils are essential dietary components, providing energy, essential fatty acids, and acting as carriers for fat-soluble vitamins. Oils and fats are composed primarily of triacylglycerols, glycerides, and both saturated and unsaturated fatty acids, and are classified as saponifiable lipids [1]. As naturally occurring long-chain fatty acid esters, they are extensively used in both industrial and household food preparations, and increased consumer demand for fried and processed foods has further expanded their usage globally [2]. Deep-fat frying is one of the oldest and most widely practiced methods of food preparation, particularly favoured for its ability to produce foods with desirable flavour, colour, and crispy texture. During frying, food is submerged in oil heated to temperatures between 150 °C and 190 °C, where simultaneous heat and mass transfer between food, oil, and air generates the characteristic and appealing sensory attributes of fried foods. Vegetable oils are widely regarded as the preferred frying medium owing to their beneficial health effects; however, their nutritional value and structural integrity are progressively compromised upon prolonged exposure to air, heat, and light [3]. Thermal oxidation, polymerization, and hydrolysis occurring during frying degrade oil quality and adversely affect the flavour and aroma of both the oil and the fried

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products prepared with it. These reactions generate volatile and non-volatile compounds that alter the sensory, nutritional, and functional properties of the frying oil [4]. Non-volatile components may additionally be absorbed by food during cooking, further accelerating oil deterioration. Prolonged use of degraded frying oils has been associated with serious health consequences, including intestinal cancers, liver damage, and atherosclerosis [2, 5, 6]. Physical changes observed during heating or frying include increased viscosity, colour darkening, and foaming [7].

Viscosity and heat transmission are key physical determinants of fried food quality, alongside factors such as food type, cooking time, temperature, and frying conditions. Several studies indicate that consumers prefer cooking oils with low viscosity, low density, and low melting points; however, higher unsaturation in such oils increases rancidity risk [8]. Repeated frying causes significant physicochemical changes through oxidation, hydrolysis, and polymerization reactions, which negatively affect oil quality and safety. Conventional analytical parameters, including peroxide value, iodine value, acid value, viscosity, and refractive index, are widely used to assess oil deterioration, though interpreting their combined influence remains challenging. Therefore, AI-based predictive analysis was incorporated in this study to examine interrelationships among physicochemical parameters and to better predict oil degradation during frying and storage [9, 10]. The primary objective of this investigation was to assess the physicochemical characteristics of various oils before and after frying and to evaluate the impact of storage duration on oil quality. Unlike earlier studies that primarily focused on a limited number of oil types or isolated analytical parameters, this work examines eleven different edible oils under standardized repeated frying and storage conditions. To the best of our knowledge, it integrates conventional physicochemical analysis with AI-assisted Random Forest predictive modelling to simultaneously evaluate oxidative, hydrolytic, and structural degradation pathways in edible oils. Additionally, the study systematically assesses the influence of storage materials, specifically transparent plastic versus coloured glass containers, on oxidative stability, providing practical and actionable insights for both industrial applications and consumer-level oil handling practices. Previous studies have evaluated physicochemical changes in edible oils during frying, but most focused on a limited number of oil types (typically two to four) or individual analytical parameters [11–13]. For example, Martín-Torres et al. [14] applied a multivariate fingerprinting approach to compare refined vegetable oils but did not incorporate AI-based predictive modelling. Tabassum et al. [12] characterised frying quality of canola and sunflower oils using conventional parameters, without examining storage material effects or predictive modelling. Yu et al. [9] and Liakos et al. [10] reviewed AI applications in food quality monitoring broadly, but no study to date has applied random forest regression to integrate multivariable physicochemical profiles of eleven different edible oils under standardised repeated frying, combined with systematic evaluation of both storage conditions (light vs dark) and storage material (transparent plastic vs coloured glass). The present study addresses this gap by providing a comprehensive, multi-oil physicochemical dataset and an AI-validated framework for identifying primary degradation markers, contributing actionable evidence for food safety monitoring and consumer guidance.

Advanced spectroscopic techniques, such as Fourier-transform infrared spectroscopy (FTIR), combined with chemometric classification, have demonstrated strong potential for rapid and non-destructive oil characterization [15]. Future research should focus on integrating these spectroscopic methods with physicochemical and AI-based analyses to achieve more comprehensive monitoring of oil quality.

MATERIALS AND METHODS

Oil samples collection

Different cooking oils including almond, soybean, sunflower, canola, sesame, mustard, coconut, olive, corn, palm olein and can olive were purchased from the local market in Lahore, Pakistan.

Frying procedure

Each oil sample (500 g) was heated to 180–190 °C in a stainless-steel deep fryer. A 50 g portion of chips (potato strips, “French fries”) was fried for 10–15 min per cycle, maintaining a food-to-oil ratio of 1 : 10 (w/w). Three successive frying cycles were conducted per oil sample. Oil temperature was monitored using a calibrated digital thermometer (± 1 °C precision). Oil samples were collected after each frying cycle and allowed to cool before analysis [14].

Physiochemical properties of oils

Peroxide value

Five grams of oil sample was added to 30 ml of chloroform-acetic acid solution (3 : 2 v/v), followed by 0.5 ml of saturated aqueous potassium iodide

(KI) solution and shaken vigorously for 60 s. Then, 30 ml of distilled water was added and shaken for 1 min. The mixture was titrated with 0.01 mol·l^{-1} sodium thiosulphate using 1% starch as an indicator, added dropwise with continuous shaking until the blue colour disappeared. A blank was run simultaneously [16]. The peroxide value (*PV*) was calculated using Eq. 1 and expressed as milliequivalents of active oxygen per kilogram of oil.

$$PV = \frac{(S - B)}{W} \times 1000 \quad (1)$$

where *S* is sample volume (in millilitres), *B* is blank volume (in millilitres) and *W* is sample weight (in grams).

Iodine value

Weigh 0.5 g of the oil sample into a measuring flask. Add 25 ml of Wijs solution (iodine monochloride dissolved in glacial acetic acid) along with 15 ml of carbon tetrachloride (CCl_4). The mixture develops a reddish-black tint. After adding 2–3 drops of 15.0% KI and stoppering tightly, the flask was kept in the dark for 1 h. Then, 15 ml of 15.0% KI and 50 ml of distilled water were added. The mixture was titrated with 0.1 mol·l^{-1} sodium thiosulfate ($Na_2S_2O_3$) using 1.0% starch as indicator until the reddish-yellow colour disappeared. A blank was titrated identically [17].

The iodine value (*IV*) was determined according to the Eq. 2

$$IV = 12.69 \times \frac{M(V_1 - V_2)}{W} \quad (2)$$

where *M* is the molarity of $Na_2S_2O_3$ (in moles per litre), V_1 is the volume used for the blank (in millilitres), V_2 is the volume used for the sample (in millilitres), and *W* is the weight of the oil sample (in grams). The value 12.69 is the conversion factor derived from the atomic weight of iodine (126.9 g·mol^{-1}) divided by 10, which converts the titrated thiosulfate volume into the equivalent mass of iodine absorbed per unit weight of oil. *IV* is expressed as grams of I_2 per kilogram of oil.

Specific gravity

Specific gravity or density of oil was measured using a pycnometer. The empty pycnometer was weighed, filled with oil sample and reweighed, then refilled with water and weighed again. Oil samples were subjected to the same procedure before and after frying. Specific gravity (SG) was calculated according to the Eq. 3 [18].

$$SG = \frac{(W_2 - W_3)}{(W_3 - W_1)} \quad (3)$$

where W_1 is the weight of the empty pycnometer, W_2 is the weight of the pycnometer filled with oil, and W_3 is the weight of the pycnometer filled with distilled water.

Refractive index

Refractive index (*RI*) was measured using a digital refractometer (Atago, Tokyo, Japan). The prism was cleaned with diethyl ether prior to use. Oil samples were filtered through filter paper to remove impurities and moisture. A few drops were placed on the prism at 40 °C, the prism closed and allowed to stabilize for 1 min before taking the reading. After recording, clean the prism with soft tissue paper before taking subsequent readings. The prism was periodically cleaned with petroleum ether and dried [20].

Moisture content

A 5 g oil sample was placed into a pre-weighed crucible. The sample was dried to constant weight in an oven preheated to 105 °C for 1 h, then cooled in a desiccator for 15 min. The moisture content (*MC*) was calculated according to Eq. 4 [19] and expressed in grams per kilogram.

$$MC = \frac{W_1}{W_2} \times 1000 \quad (4)$$

where W_1 is the loss of weight upon drying and W_2 is the weight of the oil sample.

Free fatty acid

A 5 g oil sample was weighed and transferred into a flask. Then, 100 ml of ethanol was added, followed by a few drops of 1.0% phenolphthalein indicator. The mixture was heated for 5–7 min until boiling. The solution was titrated while still hot immediately after heating against a standard potassium hydroxide (KOH) solution. During titration, the flask was shaken continuously and carefully. The titration was stopped when the solution colour changed from colourless to pink. A blank was run in parallel. The same procedure was repeated for frying samples [19].

$$AV = 56.1 \times \frac{MV}{W} \quad (5)$$

where *M* is the molarity of KOH solution (in moles per litre), *V* is the volume of KOH solution consumed during titration (in millilitres), and *W* is the mass of the oil sample (in grams). The value 56.1 represents the molecular weight of KOH. The acid value (*AV*) was calculated according to the standard method and expressed as grams of KOH per kilogram of oil.

Acid value is represented as the free fatty acid

(*FFA*) value which was calculated by the following formula:

$$FFA = \frac{AV}{2} \quad (6)$$

Saponification value

A 2 g sample of oil was poured into the flask containing 25 ml of alcoholic KOH (0.5 mol·l^{-1}) and shaken well. The mixture was heated for 60 min at 60–70 °C using a condenser that was fixed to the conical flask. To titrate the heated mixture against 0.5 mol·l^{-1} HCl until a colourless solution was obtained, two to three drops of phenolphthalein indicator (1.0%) were added. The same procedure was used to run a blank [16, 20]. Saponification value (*SV*) was calculated according to Eq. 7 and expressed as grams of KOH per kilogram of oil.

$$SV = \frac{(B - S)M}{W} \times 56.1 \quad (7)$$

where B is the volume of HCl used for the blank (in millilitres), S is the volume of HCl used for the sample (in millilitres), M is the molarity of HCl solution (in moles per litre), and W is the mass of the oil sample (in grams). The value 56.1 represents the molecular weight of KOH.

Ester value

Ester value (*EV*) of various oils was determined according to Alajtal et al. [21]. *EV* was calculated according to (Eq. 8) and expressed as grams of KOH per kilogram of oil.

$$EV = SV - AV \quad (8)$$

Viscosity

Viscosity measurements of the oil samples were carried out using an Ostwald U-tube viscometer (manufactured in Hangzhou, China). In order to keep the capillary upright, the viscometer was suspended in a water bath maintained at a constant temperature. A pipette was inserted into the side arm of the viscometer, and oil was precisely added to the mark at the top of the lower reservoir, making sure that the tube wall above the mark remained dry. After that, the viscometer was allowed to stand for a few minutes so that the sample temperature could equilibrate to the device temperature (i.e. 35 °C). Oil was transferred by suction to the other arm of the tube, raising the meniscus to a height of 1 cm above the upper reservoir's mark. The oil was let to flow freely into the U-tube, and the duration of time it took for the meniscus to move from the upper reservoir mark to the bottom reservoir mark was noted [22].

The dynamic viscosity (η) of the oil sample was calculated using Eq. 9 and expressed in centipoise.

$$\eta = \eta_0 \times \frac{\rho}{\rho_0} \times \frac{t_S}{t_0} \quad (9)$$

where η_0 is the viscosity of distilled water at the same temperature, ρ and ρ_0 are the densities of the oil and water, respectively, and t_S and t_0 are the flow times of the oil sample and distilled water.

Storage conditions

To ascertain the impact of storage conditions on the oil used in frying, 100 g of each of the eleven oil samples (almond, soybean, sunflower, canola, sesame, mustard, coconut, olive, corn, palm olein, and can olive) was taken. Potato chips were fried for 10–15 min per cycle in all the oil samples. After frying, all the oil samples were divided into two halves. One half was stored in a light-exposed area, and the second half was stored in a dark environment for 2 months. A control was run parallel, which contained oil without frying. After a specific time, *PV* was noted for all samples [23].

Storage material

Two types of bottles were used: one made of transparent plastic and the other made of coloured glass. 25 g of each oil sample, both before and after frying, were placed into each type of bottle. All bottles were stored at room temperature (25 ± 2 °C) for a period of 2 months. After 2 months, *PV* of all the samples was evaluated [24].

Artificial intelligence-based predictive analysis

To further explore the relationships among physicochemical parameters and oil degradation patterns, an artificial intelligence-based predictive analysis was performed using the experimental dataset generated in this study. The measured physicochemical parameters, including *PV, IV, AV, FFA*, η, *RI, MC* and *SG*, were used as input variables for the predictive model. The experimental dataset comprised 132 data points (11 oil types × 4 frying conditions × 3 replicates). Each data point included the measured physicochemical parameters along with frying cycle information. The dataset also incorporated frying cycle number and storage conditions as independent variables influencing oil quality. The dataset was randomly partitioned into a training subset (80 %, $n = 105$) and an independent test subset (20 %, $n = 27$). To ensure robustness and reduce overfitting on the small dataset, a 5-fold cross-validation procedure was applied to the training subset during

model development [25]. In each fold, 80 % of the training data were used to fit the model and 20 % were held out for internal validation. Model hyperparameters were tuned based on cross-validated mean coefficient of determination (R^2) and root mean square error (*RMSE*). The test subset ($n = 27$) was used exclusively for final performance evaluation and was not exposed to the model during training or cross-validation. This approach ensures an unbiased estimate of model generalization performance. Prior to analysis, the dataset was normalized to reduce variability among parameters measured in different units. A random forest regression model was applied due to its robustness in handling nonlinear relationships and multiple interacting variables [26]. The random forest model was implemented in Python (scikit-learn v1.3, INRIA, Paris, France) [27].

Hyperparameter optimization was performed using a grid search with 5-fold cross-validation over the following parameter space: number of estimators (n_estimators: 100, 200, 500), maximum depth (max_depth: 5, 10, none), minimum samples per leaf (min_samples_leaf: 1, 2, 5), and maximum features considered at each split (max_features: 'sqrt', 'log2'). The optimal configuration was: n_estimators = 200, max_depth = 10, min_samples_leaf = 2, max_features = 'sqrt'. A fixed random seed (random_state = 42) was used to ensure reproducibility.

Model performance was evaluated using statistical indicators, including R^2 and *RMSE*. Feature importance analysis was performed to determine the relative contribution of each physicochemical parameter in predicting oxidative degradation of edible oils during frying and storage. To assess the relative performance of the random forest model, three benchmark algorithms were additionally evaluated: (i) multiple linear regression (MLR) as a linear baseline, (ii) support vector regression (SVR) with a radial basis function kernel [27], and (iii) gradient boosting regression (GBR) [28]. All models were trained on the same training subset and evaluated on the same test subset under identical cross-validation conditions. Performance was compared using R^2, *RMSE*, and mean absolute error (*MAE*).

Statistical analysis

All experiments were performed in triplicate ($n = 3$), and results are expressed as mean ± standard error of the mean (*SEM*). One-way ANOVA was used to assess the effect of frying cycle on each physicochemical parameter, with Tukey's honestly significant difference (HSD) post hoc test applied where significant differences were detected ($p \leq 0.05$). Independent samples t-tests compared storage conditions and container types. Pearson correlation analysis evaluated relationships among physicochemical parameters ($p < 0.05$). All computations were performed using SPSS version 26.0 (IBM, Armonk, New York, USA).

RESULTS AND DISCUSSION

Peroxide value

PV of different oils was determined before and after frying. After frying potato chips at 180–190 °C, the *PV* increased significantly. In soybean oil, it rose from 2.75 meq·kg^{-1} before frying to 8.25 meq·kg^{-1} after the third frying. In contrast, coconut oil exhibited the smallest change, increasing from 0.64 meq·kg^{-1} to 2.19 meq·kg^{-1}. Almond, mustard, and sesame oils showed only minor increases. Overall, soybean oil exhibited the highest *PV* after frying, whereas coconut oil had the lowest value among the tested samples (Fig. 1A). The increase in *PV* across frying cycles was statistically significant for all oils (Tab. S1 in supplement). In frying applications, *PV* serves as an indicator of primary lipid oxidation, reflecting the level of peroxides and hydroperoxides, the main oxidized products of fats and oils. Repeated frying, along with the presence of moisture, accelerates the peroxidation of polyunsaturated fatty acids, resulting in progressively higher *PV* values. In the present study, all oils showed increased *PV* after the third frying, consistent with oxidative degradation during repeated heating [11, 18].

Iodine value

IV of several oil samples was assessed in the current investigation both before and after frying (Fig. 1B). The decrease in IV across frying cycles was statistically significant for all oils, with soybean and sunflower oils showing the largest absolute decreases (Tab. S2). A small difference in the decrease of *IV* of coconut oil was observed, but the reverse occurred in soybean and sunflower oil, whose values decreased to a large extent from 1284.5 g·kg^{-1} to 1109.1 g·kg^{-1} and 1330.8 g·kg^{-1} to 1126.1 g·kg^{-1} respectively. *IV* is an indicator of unsaturation and the most significant property of oils. *IV* shows the change during frying the oil at deep frying temperature, which causes the breakage of double bonds present between the fatty acid structures. In the current investigation, the value of iodine decreases with the repeated frying of oils. The breakdown of double bonds by oxidation and polymerization may be the cause of this

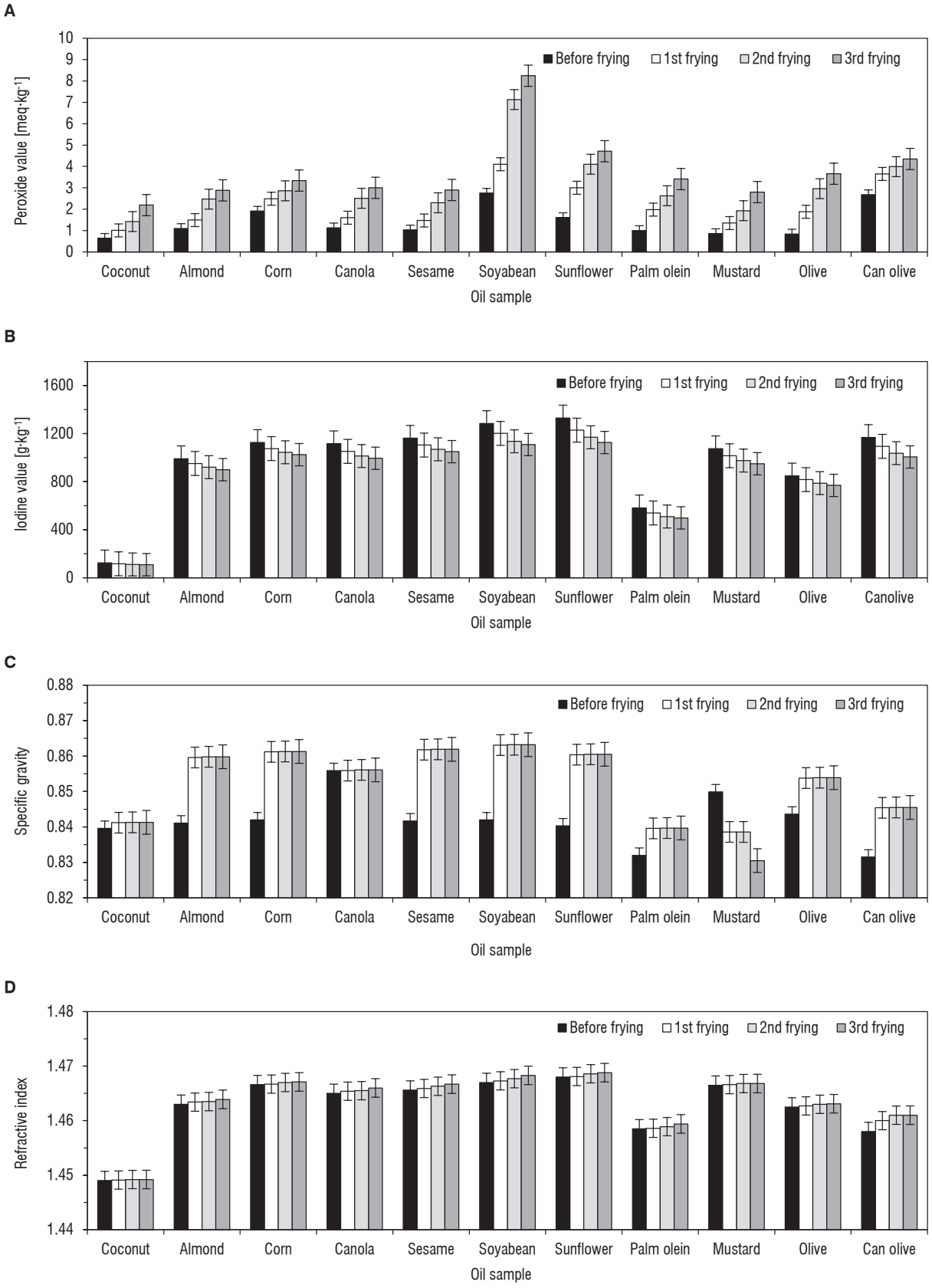


Fig. 1. Physicochemical properties of oil before and after frying.

A – peroxide value, B – iodine value, C – specific gravity, D – refractive index.
Each value is the mean of three parallel replicates. Y error bars indicate the standard error from the mean value.

decrease in *IV*. Our findings concur with those of TABASSUM et al. [12], who observed that as the frying cycle increased, *IV* of various oils decreased.

Specific gravity

In the current investigation, the *SG* of different oil samples was measured before and after frying (Fig. 1C). The results indicated an overall increase in *SG* after frying potato chips. Before frying, canola oil exhibited the highest *SG* among the tested oils at 0.8559. After the third frying cycle, soybean oil's *SG* increased from 0.8420 to 0.8632.

In contrast, mustard oil displayed a decrease in SG with repeated frying, declining from 0.8499 to 0.8305 after the third fry. *SG* serves as an effective indicator of oil purity, and generally, it increases with the fatty acid chain length. One-way ANOVA confirmed a significant effect of frying cycle on *SG* for the majority of oils tested (Tab. S3). The observed increase in *SG* after frying, except for mustard oil, can be attributed to the formation and interaction of dipoles during heating. The decrease in mustard oil may be due to its lower content of long-chain fatty acids, such as linoleic acid [12, 13].

Refractive index

In the present study, the *RI* of different oil samples before and after frying was evaluated at 40 °C. Results indicate minor changes in *RI* of all tested oils before and after frying (Fig. 1D). *RI* is the ratio between the speed of light in air (vacuum) to that in the respective sample, used to determine purity. It measures the deflection angle from one medium to another, related to the structural design of the medium and degree of unsaturation. Values may vary across different oil types, and variation is also present within the same oil type due to differences in unsaturation [29]. During deep-frying with potatoes, heat causes an increase in *RI* due to hydrogenation of unsaturated oils. In the current investigation, *RI* was determined using a simple refractometer at 40 °C. Sunflower and soybean oils showed greater *RI* values, likely attributable to hydrogenation of unsaturated fatty acids. Although the overall change was negligible, it was most pronounced after the first frying cycle. Despite this, the effect of frying cycle on *RI* was statistically non-significant (Tab. S4) for most oils, consistent with minor structural changes in unsaturation under the applied frying conditions. This supports the interpretation that *RI* is a less sensitive degradation indicator compared with *PV* and *AV* under these experimental conditions. TABASSUM et al. [12] reported the *RI* of sunflower oil as 1.466 before frying, increasing to 1.478 after frying, which aligns closely with the present study. *RI* indicates the degree of saturation in oils. There was an increase in the value of *RI* of different oil samples after frying, but the change was very small.

Moisture contents

MC of various oil samples was measured before and after frying (Tab. 1). Olive and almond oils exhibited the highest *MC* (0.70 g·kg^{-1}) before frying, while mustard (0.48 g·kg^{-1}) and palm olein (0.49 g·kg^{-1}) showed the lowest values. After the first frying cycle, olive, corn, and canola oils retained minimal moisture. By the third cycle, all samples showed negligible *MC*, indicating near-

Tab. 1. Moisture contents in different oil samples before and after frying.

Oil sample	Moisture content [g·kg^{-1}]			
	Before frying	1st frying	2nd frying	3rd frying
Coconut	0.53 ± 0.20	ND	ND	ND
Almond	0.70 ± 0.30	ND	ND	ND
Corn	0.66 ± 0.20	0.02 ± 0.10	ND	ND
Canola	0.80 ± 0.40	0.10 ± 0.10	ND	ND
Sesame	0.62 ± 0.10	ND	ND	ND
Soybean	0.61 ± 0.10	0.05 ± 0.10	ND	ND
Sunflower	0.61 ± 0.10	ND	ND	ND
Palm olein	0.49 ± 0.10	ND	ND	ND
Mustard	0.48 ± 0.20	ND	ND	ND
Olive	0.70 ± 0.10	0.03 ± 0.10	ND	ND
Can olive	0.59 ± 0.10	0.04 ± 0.10	0.01 ± 0.10	ND

The values represent mean ± standard error of the mean (n = 3). The mean difference is significant at a level of $p \leq 0.05$.
ND – not detected.

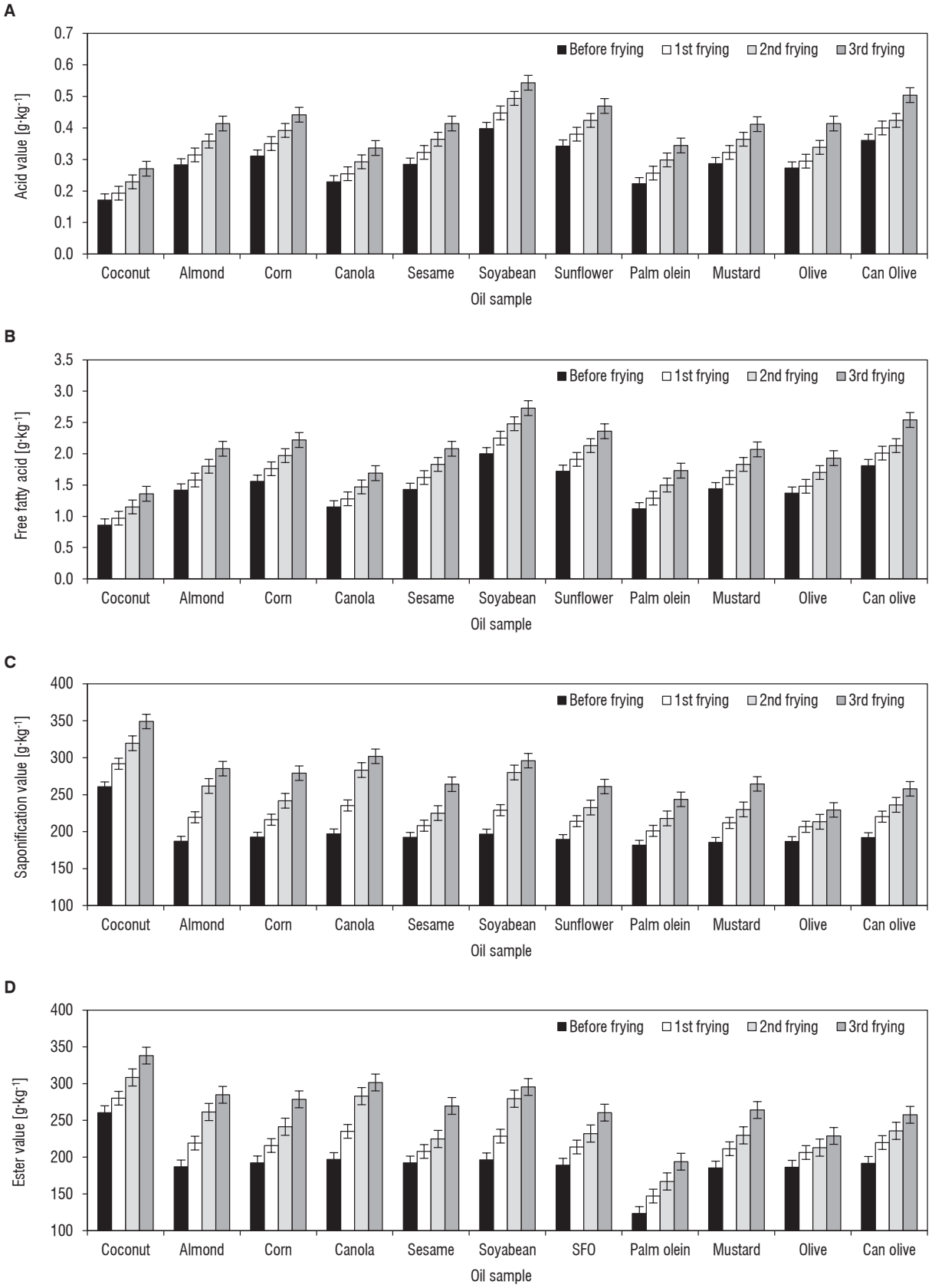


Fig. 2. Chemical quality parameters of oil before and after frying.

A – acid value, B – free fatty acid value, C – saponification value, D – ester value.
Each value is the mean of three parallel replicates. Y error bars indicate the standard error from the mean value.

complete evaporation during repeated thermal treatment. The reduction was statistically significant across all oils (Tab. 1).

Acid value

AV of different oil samples was determined before and after frying (Fig. 2A). After the third frying cycle, soybean and olive oils exhibited the highest *AV* (0.5433 g·kg^{-1} and 0.5040 g·kg^{-1}, respectively), while palm olein showed minimal change. The effect of the frying cycle on *AV* was statistically significant (Tab. S5). *AV* reflects *FFA* content, which rises due to the hydrolysis of triglycerides under high temperatures; for edible oils, values must remain below 0.6 g·kg^{-1}. Oils with higher saturated fatty acid content, such as coconut oil (rich in palmitic acid), demonstrate lower *AV* and greater oxidative stability, contributing to a longer shelf life [30]. Accordingly, coconut oil maintained low *AV* throughout frying, whereas soybean oil increased from 0.3980 g·kg^{-1} to 0.5433 g·kg^{-1}. These differences correspond to fatty acid composition, as *FFA*s are generated through thermal oxidation, hydrolysis, and pyrolysis of triglycerides [31]. Oils with elevated moisture content are additionally prone to microbial growth and quality deterioration during storage and handling [32].

Free fatty acid

FFA content of various oil samples was measured before and after frying. Soybean oil exhibited the highest *FFA* content (2.73 g·kg^{-1}) after the third frying cycle, compared to all other oils. Among the tested samples, sunflower, corn, olive, and soybean oils consistently showed higher *FFA* values both before and after frying (Fig. 2B). *FFA* and glycerol are produced via triglyceride hydrolysis, and *FFA* content serves as a key indicator of oil deterioration. Repeated frying significantly increased *FFA* levels due to the formation of carbonyl compounds and low-molecular-weight fatty acids from double bond cleavage and oxidation [33]. This increase was statistically significant across all oil types (Tab. S6).

Saponification value

The study investigates *SV* of edible cooking oils before and after frying, with results indicating notable changes across all oil samples (Fig. 2C). *SV* measures the molecular weight and triglyceride chain length of the oil and bears an inverse correlation with the average fatty acid chain length [34]. A lower *SV* reflects a lower mean molecular weight or a reduced number of ester bonds, which may suggest limited intermolecular fat interactions, whereas higher *SV* values indicate a greater proportion of low-molecular-weight fatty acids present in the oil [35]. In the present study, a gradual and consistent increase in *SV* was observed with each successive frying cycle, likely because repeated thermal treatment progressively degrades long-chain fatty acids into shorter-chain forms, thereby increasing the overall *SV* of the oil [22]. This frying-induced increase in *SV* was found to be statistically significant across all oil types examined, with coconut oil recording the highest absolute increase among all the samples tested (Tab. S7).

Ester value

EV of different oil samples was evaluated before and after frying (Fig. 2D). Coconut oil recorded the highest EV both before and after frying, while palm olein oil consistently showed the lowest values in both cases. EV is derived from SV and AV (EV = SV - AV); since SV increased more

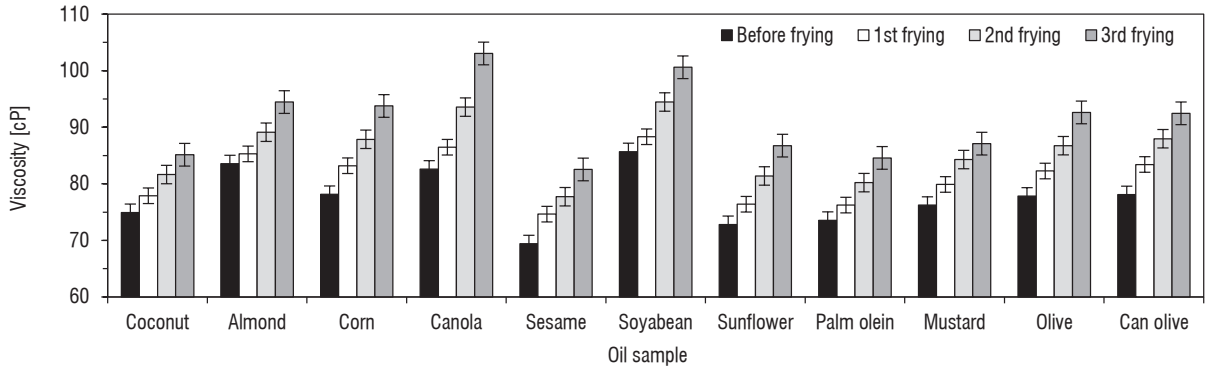


Fig. 3. Viscosity of oil before and after frying.

Each value is the mean of three parallel replicates. Y error bars indicate the standard error from the mean value.

substantially than AV with repeated frying, a net increase in EV was observed across frying cycles in most oils (Tab. S8).

Viscosity

The viscosity of several oil samples was measured before and after frying (Fig. 3). Soybean oil increased from 85.70 cP to 100.60 cP, canola oil from 82.61 cP to 103.04 cP, and sesame oil from 69.42 cP to 82.54 cP after the third frying cycle. Viscosity changed gradually during the first and second frying cycles, with a more pronounced increase observed after the third frying in all tested oils. Oil viscosity is primarily governed by triglyceride composition, as variations in fatty acid arrangement on the glycerol backbone, chain length, and degree of saturation/unsaturation are all directly linked to flow properties. Repeated frying progressively elevates *FFA* content, which contributes to increased resistance to flow. Overall, all tested oils showed a consistent increase in viscosity with repeated frying, though changes during the first two cycles remained relatively minimal. Additionally, the rise in viscosity may also result from hydrogenation of triglyceride chains or from polymerization and dimer formation during heating [36, 37]. The increase in viscosity across frying cycles was statistically significant for all oil samples, with the most pronounced changes observed after the third frying cycle (Tab. S9).

Artificial intelligence-based predictive analysis

To gain deeper insight into physicochemical relationships and oil deterioration during frying, AI-based predictive analysis was performed using the experimental data obtained in this study. The predictive model incorporated parameters including *PV, AV, IV, RI, MC*, and frying cycle number. As summarized in Tab. 2, the random forest regression model demonstrated strong predictive capability, with R^2 values ranging from 0.82 to 0.92, indicating high agreement between predicted and observed oil quality indicators. Among the evaluated variables, *PV* and frying cycle number contributed most to predicting oxidative degradation, confirming that peroxide formation is a primary and reliable marker of lipid oxidation during repeated frying cycles. *AV* and *FFA* were also significant predictors of oil deterioration, reflecting the role of hydrolytic reactions during prolonged heating. Viscosity showed a positive association with oil degradation, indicating structural changes in triglycerides and the formation of polymerized compounds – further confirming the occurrence of polymerization reactions when oils are exposed to high temperatures. *IV* demonstrated a negative relationship with *PV* and *AV*, reflecting a progressive reduction in unsaturation levels as oxidation advanced; oils with higher unsaturation were consequently more susceptible to oxidative degradation during frying. These findings confirm that multiple physicochemical parameters collectively govern oil quality deterioration. The integration of artificial intelligence analysis with conventional physicochemical evaluation provides a comprehensive approach for predicting oil degradation patterns and highlights the potential application of machine learning tools in food quality monitoring systems. This trend is consistent with previous reports indicating that unsaturated fatty acids are more prone to oxidative reactions when subjected to high temperatures. The random forest model was selected due to its robustness in handling nonlinear relationships, small datasets, and multicollinearity among physicochemical variables, and its performance was confirmed through 5-fold cross-validated grid search hyperparameter optimisation (optimal configuration: n_estimators = 200, max_depth = 10, min_samples_leaf = 2, max_features = 'sqrt'). Benchmarking against alternative models confirmed the superior performance of random forest for this dataset (Tab. S10) [26–28]. MLR achieved R^2 = 0.61 and *RMSE* = 1.14, reflecting its inability to capture nonlinear interactions among physicochemical variables. SVR

Tab. 2. Artificial intelligence-based prediction of oil degradation using physicochemical parameters.

Input parameters	AI model	Predicted indicator	R^2	*RMSE*	Feature importance [%]
Peroxide value + Frying cycle	Random forest	Oxidative degradation	0.92	0.52	34
Acid value + Free fatty acids	Random forest	Hydrolytic degradation of oils	0.88	0.56	26
Viscosity + Specific gravity	Random forest	Polymerisation level during frying	0.86	0.61	18
Iodine value + Refractive index	Random forest	Unsaturation loss	0.84	0.63	13
Moisture + Storage condition	Random forest	Shelf-life prediction	0.82	0.69	9

R^2 – coefficient of determination, *RMSE* – root mean square error.

Tab. 3. Pearson correlation coefficients *r* showing relationships among oil quality parameters.

Parameters	*PV*	*AV*	*FFA*	*IV*	Viscosity	*RI*	*MC*
PV	1.00	0.84	0.81	–0.65	0.72	0.68	0.54
AV	0.84	1.00	0.93	–0.58	0.69	0.61	0.52
FFA	0.81	0.93	1.00	–0.55	0.66	0.59	0.49
IV	–0.65	–0.58	–0.55	1.00	–0.51	–0.48	–0.32
Viscosity	0.72	0.69	0.66	–0.51	1.00	0.63	0.44
RI	0.68	0.61	0.59	–0.48	0.63	1.00	0.40
MC	0.54	0.52	0.49	–0.32	0.44	0.40	1.00

PV – peroxide value, *AV* – acid value, *FFA* – free fatty acids, *IV* – iodine value, *RI* – refractive index, *MC* – moisture content.

(RBF kernel) achieved $R^2 = 0.79$ and $RMSE = 0.83$, showing improved performance but remaining inferior to random forest. GBR achieved $R^2 = 0.89$ and $RMSE = 0.57$, closely approaching random forest performance ($R^2 = 0.92$, $RMSE = 0.52$). The superior performance of ensemble methods (RF and GBR) over linear and kernel-based approaches confirms that oil degradation involves complex, nonlinear multi-parameter interactions that linear models cannot adequately represent. Random forest was retained as the primary model due to its interpretability through feature importance scores and its robustness to small sample sizes and collinear predictors.

To substantively address the need for hybrid analytical approaches, the present study integrated two complementary analytical frameworks: conventional Pearson correlation analysis and AI-based random forest feature importance scoring. Pearson correlation quantifies linear pairwise relationships among physicochemical parameters, while random forest captures nonlinear, multivariable interactions and ranks predictors by their independent contribution to predictive accuracy. The alignment between the two frameworks, with *PV, AV*, and *FFA* consistently ranked highest in both, provides cross-validated evidence of their central role in oil degradation (Tab. 3). This dual-framework approach constitutes a hybrid analytical strategy that exploits both statistical interpretability and machine learning predictive power, providing more comprehensive insights than either method alone.

Correlation analysis

A Pearson correlation analysis was performed to determine the relationships among different physicochemical parameters of edible oils during frying; all reported correlations were statistically significant at $p < 0.05$ unless otherwise stated. The correlation matrix presented in Tab. 3 indicates strong positive relationships between *PV, AV* and *FFA* content, suggesting that oxidative and hydrolytic reactions occur simultaneously during repeated frying cycles. *PV* showed strong positive correlation with *AV* ($r = 0.84$) and *FFA* ($r = 0.81$). Conversely, *IV* showed negative correlation with *PV* and *AV*, indicating loss of unsaturation due to oxidative degradation. Viscosity also showed positive association with *PV*, reflecting polymerization reactions occurring during prolonged heating of oils. The Pearson correlations directly informed feature importance rankings in the random forest model. Parameters showing high positive correlation with *PV*, namely *AV* and *FFA*, corresponding to a combined feature importance of 26 % (*AV+FFA* group, Tab. 2), and viscosity ($r = 0.72$), contributing 18 % as part of the viscosity+*SG* predictor group, were among the highest-ranked predictors in the random forest model. The inverse relationship between *IV* and *PV* ($r = –0.65$) was reflected in the model's negative predictive weighting for unsaturation loss. This alignment between correlation analysis and AI-derived feature importance validates the robustness of both analytical approaches.

Impact of storage conditions on peroxide value

The effect of storage conditions (light vs dark) on the *PV* of various oil samples was evaluated. The results indicated that oils stored in a light-exposed environment exhibited higher *PV* both before and after frying, compared with those stored in dark conditions (Fig. 4A). Among individual oils, soybean oil showed the largest light-induced *PV* increase after the 3rd frying cycle while mustard oil showed the smallest difference (Tab. S11).

Impact of storage material on peroxide value

The effect of storage material (coloured glass bottle and transparent plastic bottle) on the *PV* of different oil samples before and after frying was evaluated. Results revealed that all oil samples

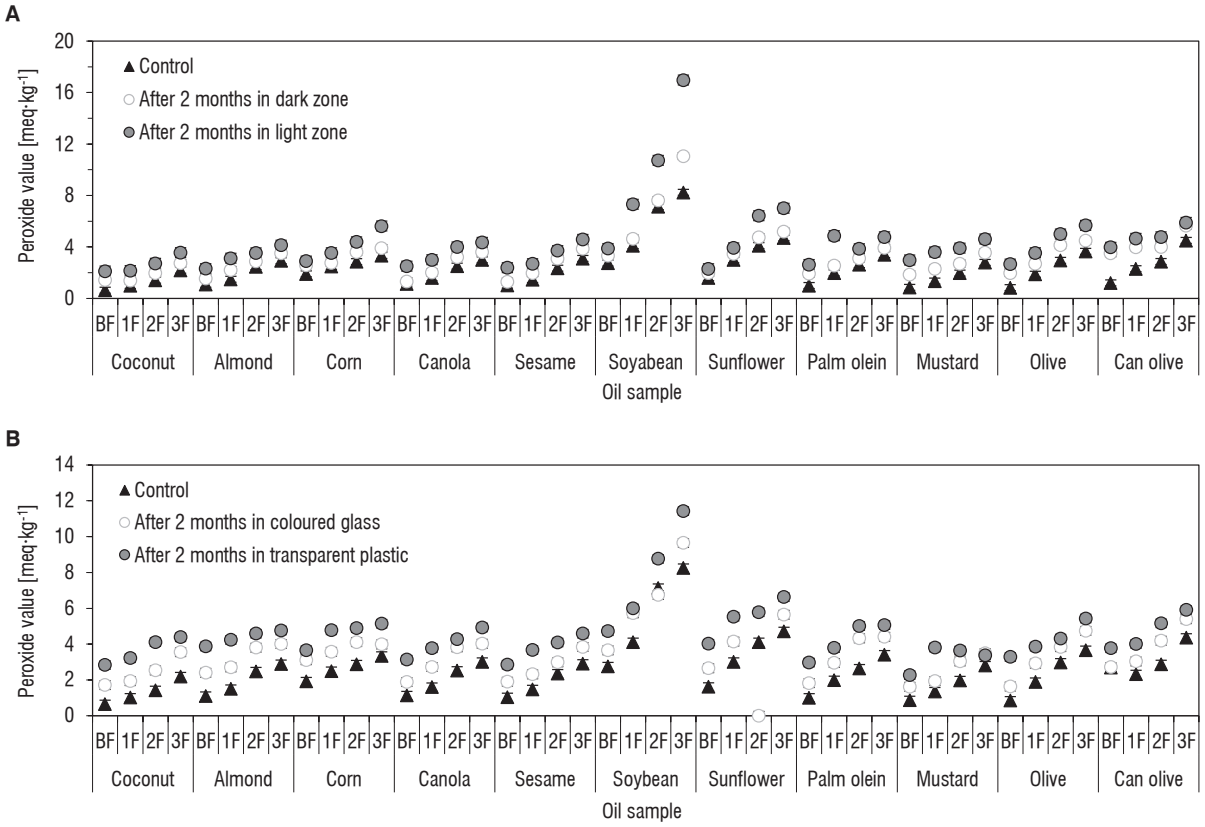


Fig. 4. Effect of storage factors on peroxide value of oil before and after frying.

A – storage conditions, B – storage material.
Each value is the mean of three parallel replicates. Y error bars indicate the standard error from the mean value.
BF – before frying, 1F – 1st frying, 2F – 2nd frying, 3F – 3rd frying.

stored in transparent plastic bottles showed higher *PV* compared to those stored in coloured glass bottles, both before and after frying (Fig. 4B). Storage conditions and duration significantly affect edible oil quality. During storage, oxidation and unsaturated fatty acids influence oil stability under both room temperature and dark storage conditions. In the present study, *PV* increased under all storage conditions, including light and dark environments and in both container types (Tab. S12). However, the increase was more pronounced in oils stored under light, likely due to light-induced oxidation. Similarly, oils stored in dark-coloured glass bottles showed smaller *PV* increases compared to transparent plastic bottles, as the latter permits greater light penetration, thereby accelerating oxidative degradation.

CONCLUSIONS

This study demonstrates that repeated frying and suboptimal storage conditions induce significant physicochemical deterioration in edible oils, characterized by increased *PV, AV, FFA* and viscosity, alongside a decrease in *IV*, reflecting the loss of unsaturated fatty acids. Oils stored in dark, coloured containers exhibited enhanced stability, underscoring the importance of proper storage practices. The integration of artificial intelligence–based predictive modelling with conventional analyses enabled accurate identification of key degradation markers (*PV, AV*, and *FFA*) providing a robust tool for rapid oil quality monitoring. The novelty lies in combining AI-assisted prediction with traditional physicochemical assessment, offering a transformative approach for real-time evaluation of frying oil safety. The random forest model, benchmarked against MLR, SVR, and GBR, achieved R^2 = 0.92 under cross-validated conditions, with *PV* combined with frying cycle number (34 %), *AV* combined with *FFA* (26 %), and viscosity combined with *SG* (18 %) as the highest feature importance weights. Integration of AI with Pearson correlation as a hybrid analytical framework provided consistent evidence for the

primacy of oxidative and hydrolytic markers in oil deterioration. These findings offer actionable insights for industry and consumers, emphasizing optimized frying practices, controlled storage, and advanced monitoring to safeguard nutritional quality and minimize health risks.

Supplementary data

Supplementary data related to this article can be found at https://www.vup.sk/download.php?bulID=2316.

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Conflict of interest

The authors declare no competing interests or financial relationships that could have appeared to influence the work reported in this paper.

Authors' contributions

Imran Ali, Roheena Abdullah, Tahreem Zahid and Afshan Kaleem investigations, data curation, data analysis, wrote first draft; Roheena Abdullah conceptualization, supervision, resources, project administration, manuscript editing and review; Roheena Abdullah, Mehwish Iqtedar and Irfana Iqbal resources, data analysis, validation, manuscript editing and review.

Data availability

All key data generated or analyzed during this study are included in this published article and its supplementary information files.

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