



Health and Sustainability Implications of Palm Oil Substitution with Platinum-Catalyzed Hydrogenated Fats in the Food Industry

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Abstract

The study conducted a comparative analysis of the quality of domestic fat and oil products obtained through hydrogenation or transesterification methods, with a focus on reducing the risk of cardiovascular diseases. The atherogenic and thrombogenic indices, as well as the ratio between hypocholesterolemic and hypercholesterolemic fatty acids, were calculated to evaluate the lipid quality of palm oil and hydrogenation products using nickel and platinum catalysts. It was found that the use of the transesterification method with palm oil (stearin) significantly reduces the content of trans-isomers. However, it simultaneously creates a more severe issue of excessive saturated fatty acid content, which significantly increases the risk of both cardiovascular and oncological diseases compared to the hydrogenation method. The solution to the problem appears to involve substituting nickel catalysts with developed low-percentage platinum hydrogenation catalysts and expediting the organization of their industrial production in the country. In this work, we have also investigated the hydrogenation mechanism of sunflower oil in the presence of a nickel catalyst by applying quantum chemical calculations and HyperChem software. The results have shown the existence of strong intermolecular interactions between linoleic acid and nickel metal according to the optimized structures, molecular electrostatic maps, molecular orbitals, bond lengths and energies.

Keywords: Palm oil; Catalyst; Fat and oil products; Spread; Margarine; Hydrogenated fat.

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1. Introduction

Palm oil has gained significant attention in recent years due to its widespread use, driven by its affordability and availability. However, ongoing research continues to evaluate its benefits and drawbacks, fueling debates on its overall impact.^[1] Known for its high resistance to oxidation, palm oil is favored for its long shelf life. Extracted from the fruit of the oil palm tree, it

is predominantly used in the food industry, especially in the production of wafers, sponge cakes, creams, and for frying semi-processed foods.^[2] Additionally, palm oil is commonly found in the processed cheese, condensed milk, blended butter, and is even added to cottage cheese-based desserts and curds. It is often used as a partial substitute for dairy fat in modern recipes. In fact, it is easier to list products that do not contain palm oil than those that do.^[3] Before discussing the benefits and drawbacks of palm oil, it is important to consider that there are several types of palm oil, varying in quality and composition.

Red palm oil is regarded as the most beneficial and natural. Its production employs a gentle technology that retains the majority of its beneficial substances. This oil exhibits a red-orange color owing to its high carotene content. Red palm oil possesses a slightly sweet taste and aroma. The beneficial properties described in the literature mainly pertain to unrefined red palm oil.^[4-6] Refined and deodorized palm oil is

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a distinct product. It lacks both odor and color, purposely processed for utilization in the food industry.^[7,8] Hydrogenated palm oil is a semi-solid substance with characteristics similar to wax or paraffin. Hydrogenated palm oil, the most inexpensive variant, is commonly used in the production of imitation products such as sour cream, cream, ice cream, and cheese. Hydrogenated fats are particularly widespread in the food industry, especially in food service, due to their enhanced heat stability. Stearin, a byproduct of hydrogenation, allows for the preparation of larger food quantities per batch while also enhancing flavor. The primary advantage of stearin is its low cost, along with other beneficial properties, such as resistance to oxidation and an extended shelf life without sacrificing quality. In its pure form, stearin is often used in candle production and is sometimes added to paraffin. Due to its negative health effects, it is recommended to avoid consuming products that contain hydrogenated palm oil. Palm stearin is also produced through fractionation.

Hydrogenation of edible oils is a chemical process used to convert unsaturated fats (found in liquid vegetable oils) into saturated fats, making the oils more solid at room temperature. This is typically done by adding hydrogen to the oil in the presence of a metal catalyst, such as nickel.^[9]

The primary purpose of hydrogenation is to improve the texture, stability, and shelf life of the oil. This process does not fully saturate the fat molecules, resulting in the formation of trans fats, which are associated with negative health effects, such as an increased risk of heart disease.^[10] Trans fats have been increasingly regulated due to these health concerns.^[11] Nickel catalysts are effective for hydrogenation but are also responsible for promoting the formation of harmful trans fats due to isomerization during partial hydrogenation.^[12] The widespread health risks associated with trans fats have led to a decline in the use of this process in favor of safer alternatives. There are several alternative catalysts to nickel for the hydrogenation of vegetable oils. These alternatives aim to reduce or eliminate the formation of trans fats, including noble metal catalysts.^[13-16]

This study focuses on a comparative analysis of the quality of fat-based products produced through hydrogenation or transesterification, with an emphasis on reducing the risk of cardiovascular diseases. The hydrogenation of sunflower oil over a nickel catalyst is also studied using quantum chemical computation. We introduce quantum chemical calculations, the PM3 method, and the HyperChem software. In particular, we investigate the optimized structures, molecular electrostatic maps, molecular orbitals, and energies of nickel-catalyzed hydrogenation of sunflower oil.

2. Materials and methods

2.1 Preparation of catalysts

Colloidal platinum was prepared by reducing hexahydrate chloroplatinic acid with NaBH₄ in the presence of polyvinyl alcohol. The sol was adsorbed onto γ -Al₂O₃, washed, filtered, and dried to obtain 0.2% Pt/ γ -Al₂O₃ catalyst. Previous studies

have thoroughly detailed the catalyst preparation process and catalyst characterization.^[17]

2.2 Catalytic hydrogenation of sunflower oil

Hydrogenation reactions were carried out in a 100 mL batch reactor (Parr 4848 autoclave, Parr Instruments, USA) equipped with a high-pressure kinetic measurement system.^[18] For each experiment, 60 mL of refined, bleached, and deodorized sunflower oil, along with 0.06 g of catalyst, were placed into the reactor. After loading, the reactor was purged with hydrogen three times to remove any air. Hydrogen was then introduced to the desired pressure once the reaction temperature was reached. The reaction was initiated by starting the agitation, and hydrogen absorption was used to monitor the process, with the final product corresponding to an iodine value of 73–76. After the hydrogenation, the catalyst was separated from the reaction products via centrifugation.

2.3 Analysis of fatty acid composition

The fatty acid composition of the initial oils and hydrogenation products was determined by gas chromatography in accordance with GOST 31754-2012 standards.^[19] Before analysis, the triglycerides were converted to their methyl esters following the procedure outlined in GOST 31665-2012.^[20] These methyl esters were then analyzed using a Chromos GC-1000 gas chromatograph (Chromos, Russia), equipped with a flame ionization detector and a CP-Sil 88 capillary column (100 m × 0.25 mm × 0.20 μ m, Agilent Technologies). Helium was used as the carrier gas, with a sample injection volume of 0.5 μ L. The fatty acid methyl esters were identified by comparing their retention times to those of the standard mixture Supelco number 19945 (FAME Mix, C4-C24).

2.4 Iodine value (IV)

The iodine value was determined in accordance with GOST R ISO 3961-2010^[21] using a refractometer (specified by GOST ISO 6320-2012) at 50 °C, based on the refractive index.^[22]

2.5 Melting point (MP)

The melting point of lard was determined following the procedures outlined in GOST 32189-2013 using the open capillary method.^[23] A capillary glass tube, open at both ends and with an internal diameter of one mm, was filled with the sample of molten lard and allowed to cool until the oil solidified at 4 °C for one hour. Afterward, the capillary containing the solidified hydrogenated fat was submerged in a water bath filled with distilled water and heated with agitation at a rate of 2 °C/min. The melting point was recorded when the oil began to move along the capillary tube.

2.6 The atherogenic index and thrombogenic index

The atherogenic and thrombogenic indices were determined based on Equations (1) and (2) as described in reference.^[24]

$$AI = \frac{4*(C14:0)+C16:0+TFA}{MUFA+(n-6)+(n-3)} \quad (1)$$

$$TI = \frac{[C14:0+C16:0+C18:0+TFA]}{[0.5*MUFA+0.5*(n-6)+3*(n-3)+(n-3)/(n-6)]} \quad (2)$$

2.7 Hypocholesterolemic (h) and hypercholesterolemic (H) fatty acids

The ratio between hypocholesterolemic (h) and hypercholesterolemic (H) fatty acids was calculated according to Equation (3):^[25]

$$h/H = \frac{C18:1+PUFA}{C14:0+C16:0} \quad (3)$$

2.8 Quantum chemical calculations

Quantum chemical calculations were performed with HyperChem software using the PM3 method to obtain optimized structures, molecular orbitals, molecular electrostatic maps, and interaction energies.

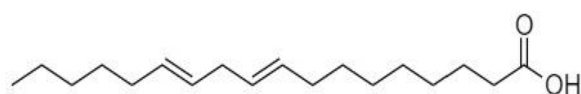


Fig. 1: Chemical structures of linoleic acid 2D.

In this regard, linoleic acid was selected as a model for calculating the fatty acid content of sunflower oil (Fig. 1).

3. Results and discussion

3.1 Palm oil analysis and hydrogenation of sunflower oil

Table 1 presents a comparison of the fatty acid composition and other characteristics of different types of palm oil, which vary in quality and constituent components.

The main component of palm oil is palmitic acid, which accounts for 40 to 73% of the product's mass. Even in animal fats, this acid is present in no more than 25-30%. Its consumption increases cholesterol levels in the body. Another

notable aspect in the analysis of palm oil composition is the low concentration of linoleic acid. This compound belongs to polyunsaturated omega-6 fatty acids. Its consumption can lower cholesterol levels and other negative effects of saturated fats. However, there is very little of it in palm oil. The consumption of palm oil, especially hydrogenated palm oil, which is present in most products, indeed leads to vascular blockages, plaque formation, and occlusion of veins and arteries. The result is atherosclerosis, thrombosis, and an increased risk of strokes and heart attacks.^[26]

Based on the fatty acid composition data, calculations were performed to determine the atherogenicity and thrombogenicity indices, which characterize the quality of lipids in palm oil and hydrogenated fats obtained by the hydrogenation of sunflower oil using nickel and platinum catalysts.^[27]

The atherogenic index indicates the ratio between the sum of major saturated fatty acids and the primary group of unsaturated fatty acids. The former is regarded as proatherogenic, promoting lipid adhesion to cells of the immune and circulatory systems, while the latter group is antiatherogenic, inhibiting aggregation and reducing levels of esterified fatty acids, cholesterol, and phospholipids, thus preventing the onset of micro- and macrocoronary diseases.^[24,26]

The thrombogenicity index indicates the tendency toward clot formation in blood vessels. It is determined by the relationship between prothrombogenic (saturated) and antithrombogenic fatty acids (monounsaturated fatty acids, polyunsaturated fatty acids ω-6, and ω-3).^[28]

The hydrogenated fats derived from sunflower oil, using both platinum and nickel catalysts, demonstrate the lowest atherogenic and thrombogenic indices. Specifically, the atherogenic index of these hydrogenated fats is 11 times lower,

Table 1: Fatty acid composition of palm oil.

Fatty Acid Content, %	Red palm oil	Refined, deodorized and bleached palm oil	Palm oil (stearin)
Lauric (C12:0)	1.1	1.5	0.1
Myristic (C14:0)	2.3	2.8	1.0
Pentadecanoic (C15:0)	-	-	0.1
Palmitic (C16:0)	45.5	33.7	72.9
Palmitoleic (C16:1)	0.2	0.2	0.1
Stearic (C18:0)	4.2	5.9	6.0
Oleic (C18:1 c)	41.5	35.5	29.9
Linoleic acid (C18:2)	9.8	16.3	5.5
Arachidic acid (C20:0)	-	0.8	0.3
Eicosenoic acid (C20:1)	-	0.4	0.03
Linolenic acid (C18:3 c2)	-	0.5	0.06
Behenic acid (C22:0)	-	0.2	0.12
Saturated fatty acids	44.9	44.8	80.8
Monounsaturated fatty acids	41.8	38.4	16.2
Polyunsaturated fatty acids	11.1	16.8	2.9
Iodine value	61.3	50-55	19.1
Melting temperature, °C	14 - 21	33 - 39	48-54

Table 2: Results of calculations for determining the atherogenicity and thrombogenicity indices, as well as the ratio between hypocholesterolemic and hypercholesterolemic fatty acids (h/H) in palm oil and hydrogenated fat obtained by hydrogenation of sunflower oil using nickel and platinum catalysts.

№	Object of study	Atherogenic index	Thrombogenic index	h/H
1	Palm oil (stearin)	2.13	8.23	0.25
2	Refined palm oil	1.28	2.21	0.81
3	Hydrogenated fat obtained by Ni catalyst	0.31	1.10	10.12
4	Hydrogenated fat obtained by Pt catalyst	0.19	1.05	9.69

and the thrombogenic index is 8 times lower compared to palm stearin. These results indicate that the high content of saturated fatty acids in palm oil substantially increases the risk of cardiovascular diseases in comparison to sunflower oil-derived hydrogenated fats. Furthermore, these hydrogenated fats display the highest ratio of hypocholesterolemic to hypercholesterolemic fatty acids (the ratio is 40 times higher compared to palm oil), further highlighting the health risks associated with the use of palm stearin.

To comparatively assess the quality indicators of the lipid phase in commercial margarines produced either through hydrogenation or transesterification with the addition of palm oil, we calculated the atherogenicity and thrombogenicity indices, as well as the ratio of hypocholesterolemic (h) to

hypercholesterolemic (H) fatty acids.

The obtained results are presented in [Tables 1 and 2](#), which provide a pairwise comparison of samples produced by hydrogenation (below) and transesterification (above).

The essence of the "palm oil issue" can be summarized as follows: the large-scale supply of cheap and low-quality types of palm oil will gradually displace domestic vegetable oils and lead to the production of a wide range of low-quality adulterated fat-and-oil and food products containing harmful palm stearin and olein, which pose health risks.^[29]

As for the prospects of further using the hydrogenation process to obtain solid fat-and-oil products, the main issue lies in the continued use of nickel catalysts. Although nickel catalysts exhibit high activity, they lack selectivity regarding

Table 3: Content of fatty acids and *trans* isomers in domestic margarines (%) purchased from local shops.

№ of product	C14:0	C16:0	C18:0	cis C18:1	trans C18:1	cis C18:2	trans C18:2	cis C18:3	SFA (%)	MUFA (%)	PUFA (%)	Σ <i>trans</i> (%)
1	0.7	31.7	5.6	30.7	1.4	28.2	0.4	0.2	38.9	32.3	28.7	1.7
2	0.2	7.1	11.8	44.2	20.4	6.4	5.1	0.9	20.2	65.7	14.1	27.2
3	0.2	8.8	10.0	44.2	25.3	7.8	2.9	0.2	19.7	69.6	10.8	28.2
4	0.6	13.4	8.2	32.7	2.9	38.0	2.0	0.4	23.1	36.4	40.5	4.9
5	1.0	35.6	4.1	32.3	0.6	24.6	0.6	0.2	41.2	33.1	25.3	1.2
6	0.4	8.7	11.3	34.6	26.4	14.9	1.80	0.9	21.1	61.2	17.7	28.2
7	0.6	12.6	11.9	45.1	6.2	18.7	0.58	2.2	26.5	51.9	21.6	6.8
8	0.4	7.9	10.6	30.3	28.9	17.9	1.55	0.3	20.4	59.9	19.7	30.5
9	1.1	45.3	3.5	38.6	0.0	10.6	0.42	0.1	50.2	39.1	10.7	0.4

SFA - saturated fatty acids (%); MUFA- monounsaturated fatty acids (%); PUFA- polyunsaturated fatty acids (%)

Table 4: Comparative assessment of the quality indicators of fat and oil products prepared using hydrogenation and transesterification methods with the addition of palm oil.

No	The sample number of margarine.	AI	TI	h/H	The sum of trans-isomers, %	The ratio of trans-isomers.	The content of FFA, %.	The ratio of SFA
1	1	0.6	1.3	1.8	1.7	15.8	38.9	1.9
	2	0.5	1.2	8.1	27.2		20.3	
2	3	0.3	0.7	5.2	4.87	5.8	23.1	1.2
	4	0.5	1.2	6.1	28.2		19.7	
3	5	0.7	1.5	1.6	1.2	22.9	41.2	1.9
	6	0.5	1.3	5.8	28.2		21.1	
4	7	0.3	0.9	5.0	6.8	4.2	26.5	1.3
	6	0.5	1.3	5.8	28.2		21.1	
5	8	1.0	2.0	1.1	0.4	72.5	50.2	2.5
	9	0.5	1.3	6.0	30.5		20.5	

cis-trans isomerization. Conducting the process at high temperatures (180-220 °C) results in a high content of trans isomers (up to 20-40% or even higher) in the hydrogenated fats (Table 3).^[30] The data presented in Table 4 were obtained by hydrogenating sunflower oil at lower temperatures (110 and 150 °C) using a nickel catalyst. The results indicate that by lowering the process temperature, the content of trans isomers can be reduced by 2-3 times. However, the trans isomer content still exceeds the requirements of the Customs Union's Technical Regulations by 6-10 times.^[31] It is also important to note that in products obtained via the hydrogenation method, even in the presence of a nickel catalyst, the saturated fatty acid content averages no more than 25-30%, which is twice as low as in fat-and-oil products containing palm oil.

0.2% Pt/ γ -Al₂O₃ and nickel (Pricat-9910) catalysts were utilized for the hydrogenation of sunflower oil at varying temperatures (90-150 °C) and a hydrogen pressure of 0.5 MPa. The catalyst-to-oil weight ratio was maintained at 1:1000, with a constant stirring rate of 800 rpm. The fatty acid compositions of the hydrogenated sunflower oil samples are shown in Table

5.

The use of palm oil reduces the level of trans isomers; however, it creates an equally serious issue-the excessive presence of saturated fatty acids, which elevates the risk of both cardiovascular and oncological diseases.^[32,33] The amount of trans fats produced using a platinum catalyst is comparable to the levels found in butter from cow's milk.

The solution to producing high-quality fat-and-oil products with low trans isomer content and without excessive saturated fatty acids (*i.e.*, without palm oil) in the country is achievable through the hydrogenation method, using innovative low-percentage (0.2% Pt) platinum catalysts (Table 4). The use of this catalyst would eliminate the need for palm oil and enable the production of hydrogenated fats with a trans isomer content of 3-6% and a saturated fatty acid content around 25%-2.5 times lower than that of palm stearin while utilizing traditional domestic vegetable oils.

The final fat-and-oil products will meet the strictest international standards. Kazakhstan has the full production capacity to process local oilseeds and produce high-quality products. To achieve this, it is essential to establish the produc-

Table 5: Fatty acid composition of hydrogenated fats obtained using Ni and Pt catalysts.

Fatty acid composition (wt. %).	Hydrogenation with Ni catalyst.		Hydrogenation with 0.2% Pt/ γ -Al ₂ O ₃ catalyst, 5 atm.	
	110 °C	150 °C	90 °C	110 °C
Myristic acid (C14:0)	0.09	0.09	0.08	0.10
Palmitic acid (C16:0)	7.17	7.37	7.04	6.90
Stearic acid (C18:0)	17.87	14.32	18.89	23.77
Oleic acid (C18:1 t6)	2.12	4.04	-	1.13
Elaidic acid (C18:1 t9)	2.69	3.94	3.81	1.84
Oleic acid (C18:1 t11)	5.40	7.41	0.93	1.24
Oleic acid (C18:1 t12)	3.08	4.35	0.39	0.57
Oleic acid (C18:1 c6)	1.93	3.10	-	-
Oleic acid (C18:1 c9)	28.60	32.00	34.55	26.09
Oleic acid (C18:1 c11)	1.06	1.56	0.83	0.77
Oleic acid (C18:1 c12)	11.33	11.59	12.38	7.21
Oleic acid (C18:1 c13)	0.23	0.45	0.17	0.17
Oleic acid (C18:1 c15)	0.15	0.50	0.08	0.09
Linolelaidic acid (C18:2 t)	0.76	0.98	0.23	0.40
Linoleic acid (C18:2 t9c12)	0.80	0.51	0.30	0.34
Linoleic acid (C18:2 c9 t12)	0.53	0.30	0.18	0.17
Linoleic acid (C18:2 c9 c12)	14.70	5.81	18.60	27.80
Arachidic acid (C20:0)	0.30	0.32	0.32	0.30
Eicosenoic acid (C20:1)	0.22	0.18	0.10	0.12
Linolenic acid (C18:3 c2)	0.16	0.19	0.14	0.18
Behenic acid (C22:0)	0.67	0.80	0.79	0.69
Lignoceric acid (C24:0)	0.19	0.22	0.28	0.21
C18:1 trans-isomers	13.28	19.74	5.13	4.77
Σ trans-isomers (%)	15.36	21.52	5.84	5.68
Iodine value, g I ₂ /100g	78.27	73.06	79.52	83.85
Melting point (°C)	46.0	37.4	39.10	46.4
Saturated fatty acids	26.30	23.11	27.41	32.00
Monounsaturated fatty acids	56.77	69.11	53.15	39.16
Polyunsaturated fatty acids	16.93	7.78	19.45	28.89

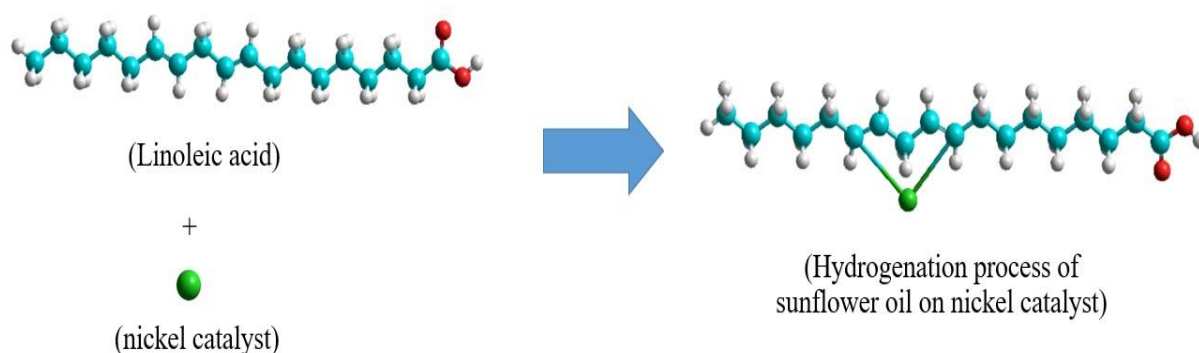


Fig. 2: Optimized structures of linoleic acid, nickel catalyst and the complex of linoleic acid with nickel. Color key: gray: hydrogen; green: carbon; red: oxygen; green: nickel.

tion of selective low-percentage platinum hydrogenation catalysts, which help reduce trans isomer levels. Unlike nickel catalysts, platinum catalysts can be reused 2-3 times, making them more efficient.^[17,34]

3.2 Insight into the hydrogenation of sunflower oil at the atomistic level

In this work, linoleic acid, nickel catalyst, and the complex of linoleic acid with nickel were studied in order to understand the process of hydrogenation of sunflower oil on a nickel catalyst using quantum chemical calculations. Optimized structures, molecular electrostatic maps, molecular orbitals and energies were calculated for linoleic acid, nickel and the complex of linoleic acid with nickel using quantum chemical calculations. Nickel metal was coordinated in our calculations through the unsaturated part of linoleic acid (containing double bonds) (Figs. 2-4).

The structures initially optimized for linoleic acid, nickel, and the linoleic acid complex with a nickel catalyst are depicted in Fig. 2. It can be clearly seen that nickel acts as a coordinating agent with the unsaturated (double bond) side of linoleic acid. Moreover, the short distances between nickel and linoleic acid were 3.74 Å and 3.49 Å, respectively.

Second, molecular electrostatic maps of the optimized geometrical structures of pure linoleic acid, nickel, and the complex of linoleic acid with nickel were studied in detail. Fig.

3 shows the results of molecular electrostatic maps of linoleic acid, nickel and the complex of linoleic acid with nickel. It can be noted that charges are localized around nickel with linoleic acid.

Third, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) molecular orbitals were illustrated for the optimized structures of linoleic acid, nickel, and the nickel complex with linoleic acid. Fig. 4 shows the HOMO-LUMO results of linoleic acid, nickel and the complex of linoleic acid with nickel. In Fig. 4, it can be noted that the HOMO and LUMO are located around the unsaturated double bond group of linoleic acid bound to nickel. Moreover, the HOMO energy was -9.42 eV, while the LUMO energy was 0.66 eV. Therefore, the difference between HOMO energy and LUMO energy is high, which can prevent the catalyst from chemically reacting and increase the rate of hydro-generation reaction of sunflower oil.

Fourth, the total energy of linoleic acid was -74160.5 kcal/mol, and the total energy of nickel was -23810.1 kcal/mol, and the total energy of the complex of linoleic acid with nickel was -98014.2 kcal/mol. Here, the bond energy (E_{bond}) of this catalytic process can be calculated as follows: $E_{\text{bond}} = -98014.2 \text{ kcal/mol} - (-23810.1 \text{ kcal/mol} - 74160.5 \text{ kcal/mol}) = -43.6 \text{ kcal/mol}$. In this regard, E_{bond} , as observed in the above calculation, indicates the preferential catalytic activity of the nickel catalyst for the hydrogenation of sunflower oil.

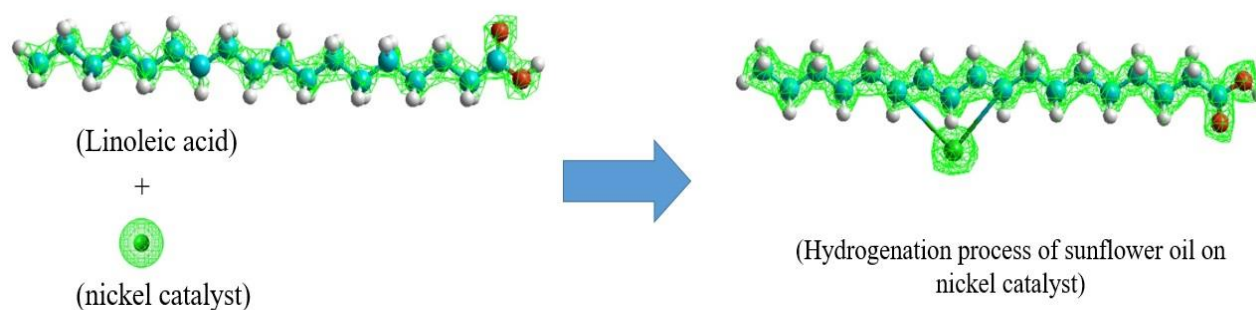


Fig. 3: Molecular electrostatic maps of linoleic acid, nickel and the complex of linoleic acid with nickel.

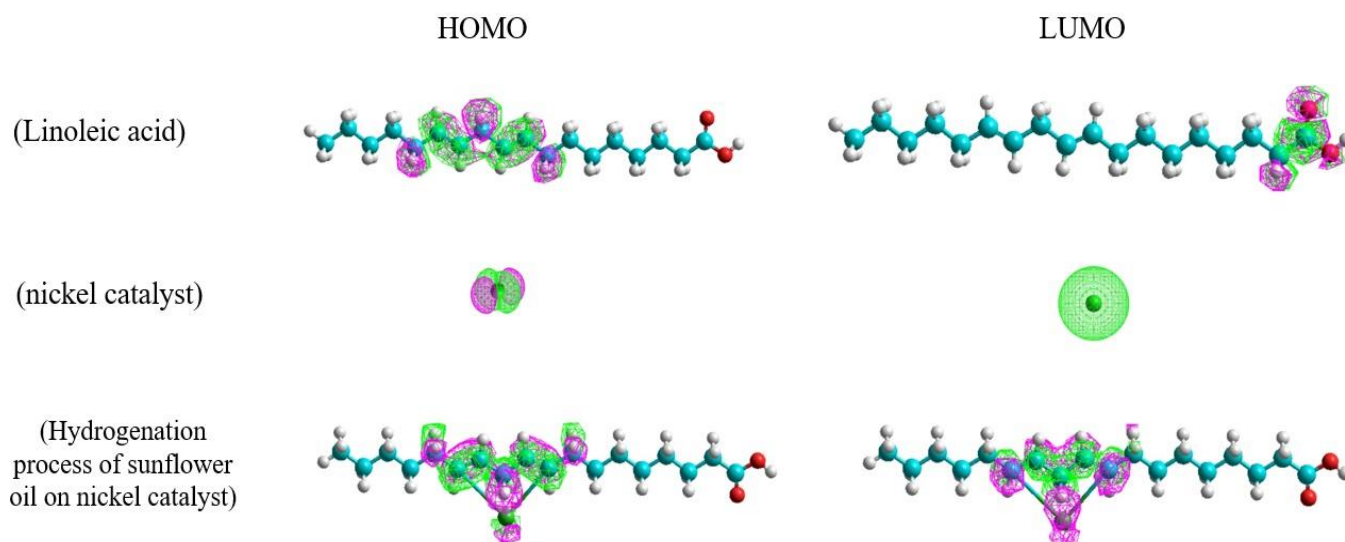


Fig. 4: Highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) of linoleic acid, nickel catalyst, and complex of linoleic acid with nickel catalyst.

4. Conclusion

The results unequivocally demonstrate that substituting traditional hydrogenation methods with transesterification using palm oil does not provide a viable solution for producing high-quality fat-and-oil products. While reducing the trans isomer content to 2% through transesterification complies with the Customs Union Technical Regulation TR CU 024/2011-implemented to benefit palm oil suppliers, this approach has resulted in an influx of counterfeit butter, spreads, and margarines containing high levels of palm stearin, along with food products derived from them. The solution to this issue involves replacing nickel catalysts with our proposed selective low-percentage platinum catalysts and expediting the establishment of their industrial production. In this work, we also investigated the mechanism of hydrogenation of sunflower oil in the presence of a nickel catalyst by applying quantum chemical calculations and HyperChem software. In conclusion, the process of hydrogenation of sunflower oil using a nickel catalyst was modeled by quantum chemical calculations. The complex of linoleic acid with nickel was chosen as the calculation model of the sunflower oil hydrogenation process. The result of quantum chemical calculation showed that nickel linoleic acid has a low coordinate bond energy and a high HOMO-LUMO energy difference with the unsaturated double bond side.

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Conflict of Interest

There is no conflict of interest.

Supporting Information

Not applicable.

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