Development of software for the determination of the thermodynamic properties of biodiesel

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Resumen

El diseño, operación y simulación de plantas industriales de producción de biodiesel requiere el conocimiento de las propiedades termodinámicas de los diferentes componentes que participan en la conversión de aceites vegetales. En este trabajo se desarrolló un programa para determinar entropía, entalpía, capacidad calorífica y energía libre de Gibbs tanto para los ácidos grasos en el aceite como para los ésteres en el biodiesel. La determinación de las propiedades se realizó con base en cuatro diferentes métodos de contribución de grupos. Los resultados se verificaron con datos experimentales obtenidos de literatura. El objetivo fue el desarrollo de un software de uso práctico y accesible que puede usarse para una amplia variedad de ácidos grasos y ésteres metílicos o etílicos desde C_{12} a C_{24}. Además, el software presenta la determinación de las propiedades termodinámicas estándar de los ácidos carboxílicos contenidos en 7 diferentes aceites: jatropha, canola, girasol, algodón, palma, oliva y soya. Estos aceites son los más usados para producir biodiesel, y así el programa desarrollado puede aplicarse ampliamente a la industria de biodiesel. Al considerar las propiedades individuales de cada componente triglicérido en el aceite se puede simular la conversión específica de estos 7 aceites vegetales, lo cual no ocurre en un simulador comercial.

Palabras clave—Aceite, biodiesel, contribución, termodinámica, programa.

Abstract

The design, operation and simulation of industrial biodiesel production plants require knowledge of the thermodynamic properties of the different components involved in the conversion of vegetable oils. In this work, a program was developed to determine the entropy, enthalpy, heat capacity and Gibbs free energy for both fatty acids in oil and esters in biodiesel. The determination of the properties is carried out on the basis of four different methods of group contribution. The results were verified with experimental data obtained from the literature. The objective was to develop practical software that can be used for a wide variety of fatty acids and methyl or ethyl esters from C_{12} to C_{24}. In addition, the software presents the determination of the standard thermodynamic properties of carboxylic acids contained in 7 different oils: jatropha, canola, sunflower, cotton, palm, olive, and soybean. These oils are the most widely used oils to produce biodiesel; thus, the developed program can be widely applied in the biodiesel industry. By considering the individual properties of each triglyceride component in the oil, the specific conversion of these 7 vegetable oils can be simulated, which does not occur in a commercial simulator.

Keywords*— Biodiesel, oil, contribution, thermodynamics, software.*

1. INTRODUCTION

In Mexico, petroleum production has declined significantly since 2004, when it reached its peak [1], and at the same time, the demand for clean and renewable energies has increased. Therefore, it is necessary to look for new alternatives to meet the country's energy needs. Biofuels, such as biodiesel, represent promising alternatives to renewable energy.

In the design of equipment, operation, simulation and optimization of biodiesel production plants, thermodynamic data of the components involved in the biodiesel reaction are needed. However, these data are not reported in the literature, specifically for a type of vegetable oil, so it is common to use thermodynamic data of model molecules for both oil and biodiesel. This does not correspond to the real properties of the mixture of components contained in vegetable oil, animal fat or biodiesel.

By knowing the composition and molecular structure of the predominant components in both vegetable oil and biodiesel, it is possible to apply group contribution methods to estimate their thermodynamic properties. Knowledge of the thermodynamic properties of biodiesel is crucial for determining the energy balance in biodiesel reactors, which is required in the design and optimization of the process. Thermodynamic properties influence the combustion process and, therefore, the emissions produced, impacting environmental sustainability[2].

A number of authors[3–11] have previously estimated the thermodynamic properties of vegetable oils and biodiesel components via group contribution methods. For instance, Cunico et al.[4] used four methods to estimate the boiling temperature, critical temperature, critical pressure, critical volume, Gibbs energy of formation, enthalpy of formation, acentric factor and liquid heat capacity of twenty-two fatty acids (C_4 to C_{20}) and their corresponding methyl and ethyl esters and eight vegetable oils and their respective biodiesels. Compared with the experimental data, the average relative deviations (ARD%) of their results are between 0.13 and 11.24%. Rabelo-Silva et al. [7] created a database for estimating the thermophysical properties of vegetable oils and evaluated the performance of group contribution methods. The absolute average relative deviation in the determination of the standard energy of formation for glycerides (tri-di and mono-) was 0.954%, 0.754% and 2.733% for the Joback, Gani and Benson methods, respectively. Similarly, Cruz-Forero et al.[10] calculated the thermophysical properties (calorific capacity, density, viscosity, boiling temperature, and vapor pressure) of three vegetable oils (soybean oil, canola and olive) and their triglycerides via an extended constituent fragment method. They compared their estimated values with those calculated with Aspen Plus software. The average relative errors were between 1% and 32%, depending on the property.

The implementation of the equations developed by these authors is relatively complex, as there is still a significant need for programming before its practical application. On the other hand, simulators such as ASPEN Plus and SuperPro Designer determine a limited number of properties, but they have a high cost for use in industry or for a single user. Thus, the main objective of this work is to develop a program that is affordable to the public and industry to accurately determine the properties of the compounds involved in the production of biodiesel.

As an innovation, unlike the methods that the above authors have developed or applied, we used for the first time the method of Domalski and Hearing [12] to biodiesel industry-related compounds. The scope of this work is the estimation of the entropy, enthalpy and heat capacity for methyl, ethyl and carboxylic acid esters from C_{12} to C_{24} and their parent try- and monoglycerides.

From the value of these properties, the program estimates the heat of combustion and the heat capacity for different types of vegetable oils and their corresponding biodiesel, as well as the enthalpy of reaction at different reaction temperatures.

2. METHODOLOGY

Jatropha curcas L. oil was supplied by the Centro de Desarrollo de Productos Bióticos (CEPROBI-IPN) in Mexico, whereas Canola oil (pure) was purchased from a supermarket. The fatty acid composition of both oils was analyzed by gas chromatography (GC), and the corresponding fatty acid methyl ester composition in weight percent (wt.%) was determined by their derivation following a modified method, AOAC 969.33, by Lee et al.[13]. Additionally, the compositions of 6 other vegetable oils (olive, palm, sunflower, castor, cotton and soybean) were collected from the literature [14–17]. The composition of the oils for the derived methyl esters was taken as a basis for estimating the composition of the parent triglycerides and fatty acids. For the latter, the concentration of free fatty acids was also considered.

The method of Domalski and Hearing [12] was used for estimating the thermodynamic properties in the liquid phase. This method extends the group contribution method of Benson for the estimation of the properties of liquid and solid organic compounds containing oxygen, such as fatty acids and esters.

Since biodiesel and oil are in a liquid state during processing in the biodiesel industry, determining their properties in the liquid phase is important. Therefore, the Domalski et al. method was used to develop a program to calculate the standard enthalpy of formation at 298.15 K, heat capacity, entropy of formation, Gibbs free energy, heat of reaction and heat of combustion of triglycerides, diglycerides, monoglycerides, fatty acids, methyl esters and ethyl esters, from C_{12} to C_{24}. The program was written in Java.

Java is a statically typed object-oriented programming language and a platform-independent language that runs on any operating system. Primitive data types are passed by value, whereas objects are passed by reference. The flowchart of the algorithm is shown in Figure 1.

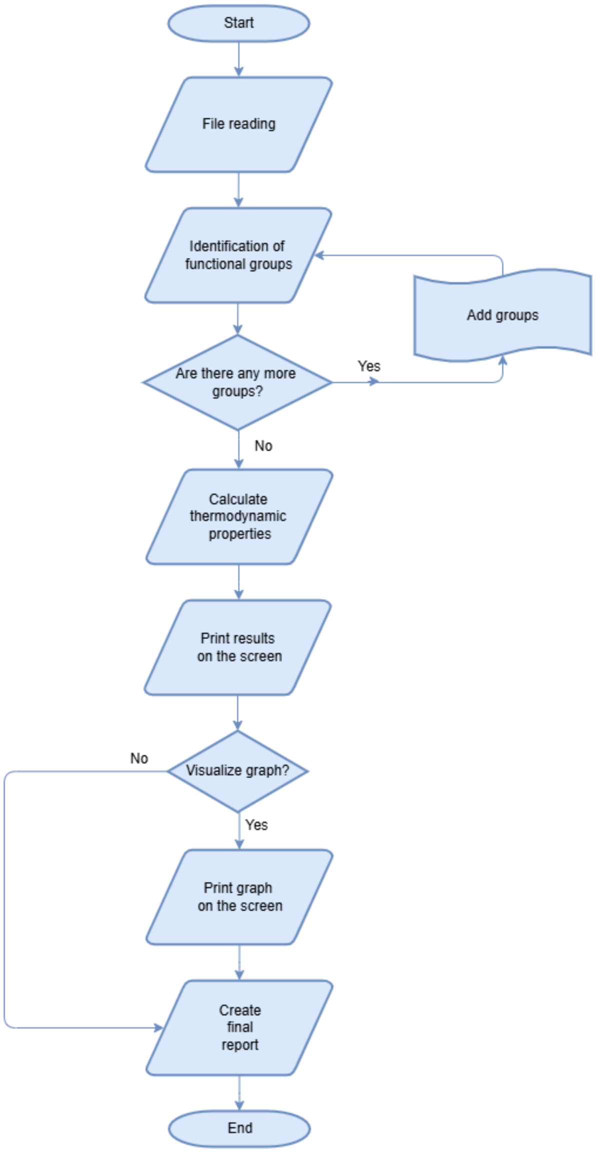


Figure 1. Algorithm flowchart of the program

The main screen of the program contains menus for triglycerides, fatty acids, methyl esters, ethyl esters, and biodiesel.

The architecture of the program is shown in Figure 2. It is a variation of the Model–view–controller software design pattern where the user is presented with a graphical user interface where she can select a compound and press the init button. The thermodynamic properties are calculated and sent to a text box in the graphical user interface, where they can be copied. Afterwards, the visualization button is activated so that the user can optionally press it; this will create a visualization in a new window of the molecule (see Figure 3). The module that calculates the thermodynamic properties and the module that creates the visualization have nothing in common, other that they work with the same text file with the information from the compound.

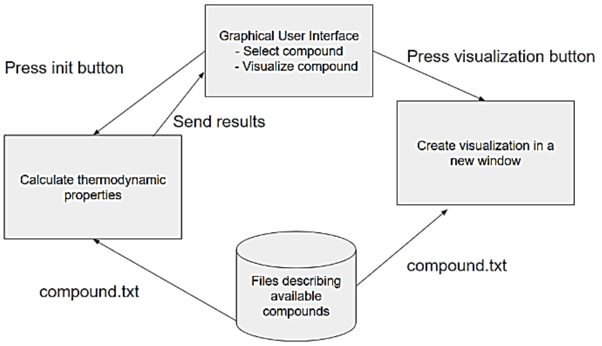
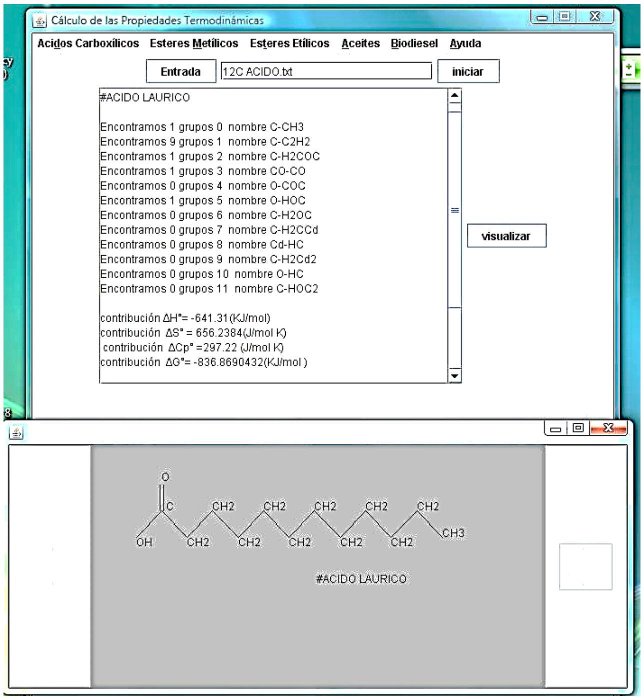


Figure 2. Architecture of the program

Visualization of the chemical structure of each compound enhances the user´s understanding of its characteristics.



```
#ACIDO LAURICO

Encontramos 1 grupos 0  nombre C-CH3
Encontramos 9 grupos 1  nombre C-C2H2
Encontramos 1 grupos 2  nombre C-H2COC
Encontramos 1 grupos 3  nombre CO-CO
Encontramos 0 grupos 4  nombre O-COC
Encontramos 1 grupos 5  nombre O-HOC
Encontramos 0 grupos 6  nombre C-H2OC
Encontramos 0 grupos 7  nombre C-H2CCd
Encontramos 0 grupos 8  nombre Cd-HC
Encontramos 0 grupos 9  nombre C-H2Cd2
Encontramos 0 grupos 10  nombre O-HC
Encontramos 0 grupos 11  nombre C-HOC2

contribución ΔH°= -641.31(KJ/mol)
contribución  ΔS° = 656.2384(J/mol K)
 contribución  ΔCp° =297.22 (J/mol K)
contribución  ΔG°= -836.8690432(KJ/mol )
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Figure 3. An example of the execution of the program

To validate the results, the formation enthalpy and entropy of triglycerides were compared with the experimental values reported in the NIST Chemistry Webbook [18].

As an illustration of the program's application, the energy balance of a transesterification reaction in a batch reactor was determined.

3. RESULTS AND DISCUSSION

3.1. Vegetable oil composition. The compositions of the vegetable oils studied in this work are shown in Table 1. Most oils contain significant amounts of oleic and linoleic acids. We can infer that most of the studied oils are composed of high concentrations of triolein and trilinolein, except for palm and castor oils, which are characterized by significant amounts of tripalmitin and triricinolein, respectively.

Table 1. Fatty acid composition of vegetable oils (wt.%)

Fatty acids	Structure	Jatropha	Canola	Sunflower	Cotton	Palm	Olive	Castor	Soybean
Myristic	C14:0	0.13			1.00	1.80	0.01		
Palmitic	C16:0	12.76	3.65	6.45	22.90	41.10	13.78	1.60	8.36
Palmitoleic	C16:1	0.61	0.18		0.60	5.00	1.36		
Stearic	C18:0	7.46	1.65	4.84	3.40		2.41	0.90	3.36
Oleic	C18:1	43.89	63.72	21.67	19.40	40.00	68.27	3.00	23.62
Ricinoleic	C18:1 OH							89.50	
Linoleic	C18:2	34.78	15.42	66.36	52.20	11.00	12.68	4.00	57.79
Linolenic	C18:3	0.29	14.28	0.68	0.50	0.30	0.74		5.55
Arachidic	C20:0		1.10			0.80	0.40	0.40	0.70
Eicosenoic	C20:1	0.08					0.25		0.62
Behenic	C22:0						0.10	0.60	

Data taken from refs. [14–17].

3.2. Calculation of the standard formation properties. The software provides the thermodynamic properties of triglycerides via the Benson group contribution method improved by Domalski and Hearing [12]. For example, triolein has the molecular structure shown in Figure 4.

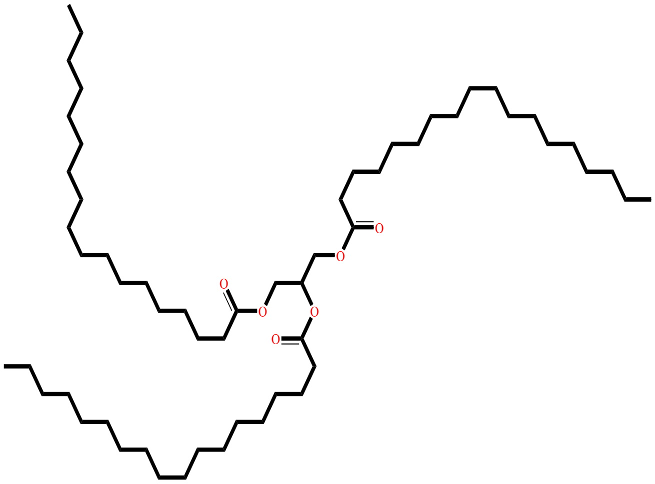

Figure 4. Chemical structure of triolein

Once the structure is known, the number of each group can be determined and multiplied by the corresponding thermodynamic property value, as shown in Table 2, for triolein. To estimate S° (298.15 K), the contributions are added, and ΔS is then calculated by including the symmetry and isomer corrections as follows:

$$S^{\circ}\,(298\text{ K}) = \sum_j n_j \Delta_s - R\ln\sigma + R\ln\eta \qquad (1)$$

where σ is the symmetry number and η is the number of possible optical isomers. For $\Delta H°f$ (298.15 K) and $Cp°(T)$, symmetry or optical isomer corrections are not needed.

Table 2. Calculation of the thermodynamic properties of triolein.

Contributions	No	$\Delta H_f°_{(L)}$ (Kj/mol)	Cpº (298K) (J/mol K)	Sº (298K), (J/mol K)
$C\text{-}CH_3$	3	3(-47.61)	3(36.48)	3(83.30)
$C\text{-}H_2C_2$	33	33(-25.73)	33(30.42)	33(32.38)
$C\text{-}H_2CCd$	6	6(-25.73)	6(29.29)	6(31.67)
Cd-HC	6	6(31.05)	6(24.60)	6(28.58)
$C\text{-}H_2COC$	3	3(-24.14)	3(29.29)	3(39.87)
CO-CO	3	3(-149.37)	3(44.98)	3(32.72)
O-COC	3	3(-196.02)	3(19.58)	3(38.28)
$C\text{-}H_2OC$	2	2(-35.80)	2(33.64)	2(32.59)
$C\text{-}HC_2O$	1	-27.60	49.83	-29.08
Total	60	-2167.79	1835.3	2048.65

Applying the symmetry and isomer corrections, Eq. (1), to the total value of S° results 2021.25 J/mol K. To determine the entropy of formation, it is necessary to know the components that make up the chemical compound. Then, with Eq. (2), given by Domalski and Hearing [12], $\Delta S^0{}_f$ can be calculated:

$$\Delta S^0{}_f = C\,(0.690R) + H\,(15.7041R) + O\,(24.6604R) \times S^0 \; (2)$$

where:
C = number of carbon atoms present in the compound.
H = number of hydrogen atoms present in the compound.
O = number of oxygen atoms present in the compound.
S^0 = standard entropy of the compound, determined via the program.
R = ideal gas constant: $8.314\ J/mol\ K$

Once the enthalpy and entropy of formation are known, at the desired temperature T, the Gibbs free energy can be determined as follows:

$$\Delta G^0{}_f = \Delta H^0{}_f - T\,\Delta S^0{}_f \qquad (3)$$

where:
$\Delta G^0{}_f$ = standard Gibbs free energy of formation
$\Delta H^0{}_f$ = standard enthalpy of formation
$\Delta S^0{}_f$ = standard entropy of formation

Similarly, the properties of fatty acids and methyl- and ethyl-esters were calculated.

3.3 Calculation of heat capacity at a given temperature

The Benson group contribution method was used to determine the Cp value from a temperature range between 300 and 1000 K. The Cp values were obtained via the following equation:

$$C_p{}^{\circ}\,(T) = a + bT + cT^2 + dT^3 \qquad (4)$$

The coefficients a, b, c and d for each compound were determined by the group contributions. Tables 3 and 4 show the regressed parameters for triglycerides and methyl esters, respectively.

Table 3. Estimated coefficients for the Cp calculation of triglycerides

Triglyceride	a	b	c	d
Tripalmitin	34.206463	4.750784	-2.610305E-3	5.032438E-7
Tripalmitolein	66.44955	4.440573	-2.293295E-3	3.697062E-7
Tristearin	28.224283	5.323442	-2.940335E-3	5.765116E-7
Triolein	60.467406	5.013231	-2.623326E-3	4.429741E-7
Trilinolein	26.814078	5.022464	-2.794164E-3	5.439898E-7
Trilinolenin	-6.839204	5.031698	-2.965004E-3	6.450055E-7

Table 4. Estimated coefficients for the Cp calculation of methyl esters

Methyl ester	a	b	c	d
Methyl palmitate	29.677382	1.50593	-7.378913e-4	1.076907e-7
Methyl palmitoleate	40.425076	1.402526	-6.322214e-4	6.317829e-8
Methyl stearate	27.683322	1.696816	-8.479014e-4	1.321133e-7
Methyl oleate	38.431016	1.593412	-7.422313e-4	8.760089e-8
Methyl linoleate	27.391439	1.606678	-7.628271e-4	1.382465e-7
Methyl linolenate	16.3516982	1.61978937	-9.291833e-4	1.8889197e-7

Tables 4 and 5 show the estimated values for triglycerides and methyl esters, respectively. The properties of the ethyl esters were determined in the same way.

Table 5. Thermodynamic properties estimated for triglycerides

TG/Property	ΔH_f^O (Kj/mol)	S^O (J/mol K)	Cp^O (J/mol K)	ΔH_C (Kj/mol)	Cp(333K) (J/mol K)	Mw
Tripalmitin	-2354.09	1853.28	1694.48	-31724.14	1345.35	806
Tripalmitolein	-2013.41	1826.22	1652.78	-31207.30	1304.51	800
Tristearin	-2508.47	2047.56	1877.00	-35646.22	1496.17	890
Triolein	-2167.79	2020.50	1835.30	-35129.38	1455.33	884
Trilinolein	-1823.21	1958.52	1831.76	-34616.44	1409.54	878
Trilinolenin	-1478.67	1896.54	1828.22	-34103.46	1363.75	872

Table 6. Thermodynamic properties of methyl esters.

Ester/Property	ΔH_f^O (Kj/mol)	S^O (J/mol K)	Cp^O (J/mol K)	ΔH_C (Kj/mol)	Cp(333K) (J/mol K)	Mw
Methyl palmitate	-799.24	671.008	562.27	-10750.73	453.3046	270
Methyl palmitoleate	-685.68	661.988	548.37	-10578.45	439.6929	268
Methyl stearate	-850.70	735.768	623.11	-12058.09	503.5785	298
Methyl oleate	-737.14	726.748	609.21	-11885.81	489.9670	296
Methyl linoleate	-622.28	706.0884	608.03	-11714.83	482.93097	294
Methyl linolenate	-507.42	685.428	606.85	-11543.85	397.7490	292

A comparison of the calculated formation enthalpy, entropy and standard heat of combustion of triglycerides with the available experimental values reported in the NIST Chemistry Webbook revealed that the AAD was between 1.6 and 6.2%, which are between is a reasonable value to use the program with certainty.

3.4. Calculation of the thermodynamic properties of biodiesel

The composition of biodiesel from different vegetable oils was first calculated in terms of mole fractions. An ideal mixing rule was then used to estimate the value of each thermodynamic property. As vegetable oils are commonly transesterified at 333.15 K, the heat capacity was also determined at this temperature (see Table 7). In addition to the properties shown in Table 7, the enthalpy of combustion was also estimated for biodiesel.

The heats of combustion for biodiesel-related compounds are not currently available in the literature, but these values are critical to the modeling of the combustion chemistry of the subject compounds[18].

Table 7. Estimated properties of biodiesel from different vegetable oils.

Property: Biodiesel from:	ΔH_f^O (KJ/mol)	S^O (J/mol K)	Cp^O (J/mol K)	Cp^O (333 K) (J/mol K)	ΔH_C (KJ/mol)
Jatropha	-714.278	712.486	603.316	483.4371	-39.67
Canola	-693.306	715.307	606.517	477.5162	-40.017
Olive	-733.824	715.043	600.5827	482.5907	-40.062
Palm	-753.4352	696.779	547.760	471.0760	-39.957
Soybean	-669.293	705.443	602.9768	474.2850	-39.908
Cotton	-696.366	703.158	598.2567	478.3020	-39.929
Sunflower	-675.493	710.231	605.936	483.7021	-39.955

3.5. Thermochemistry of the transesterification reaction.

Once the values of the properties shown in Tables 5, 6 and 7 are known for several mixtures, it is possible to calculate the thermochemistry of the corresponding alkaline transesterification reaction (see Figure 5), including the standard reaction enthalpy, reaction heat capacity and reaction entropy, as shown in Table 8.

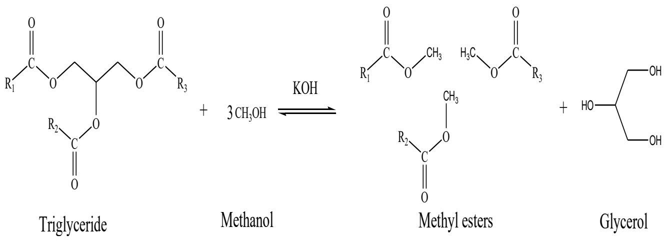

Figure 5. Transesterification reaction with potassium hydroxide as a catalyst

Table 8. Thermodynamic reaction properties

Property/Vegetable oil	ΔH_R^O (KJ/mol)	Cp^O_R (J/mol K)	Cp^O_R (333 K) (J/mol K)	S^O_R (J/mol K)
Jatropha	0.264	-84.1795	8.442	-54.9766
Canola	0.9455	-85.1178	-13.9598	-56.0752
Olive	-0.222	-83.7951	2.3373	-54.5676
Palm	-0.438	-198.3657	3.3576	-54.385
Soybean	-8.5428	-75.3895	4.14196	-45.5560
Cotton	-9.5E-3	-83.9778	13.2459	-54.5595
Sunflower	-0.424	-84.225	15.4331	-55.0415

3.6. Application to model a reactor batch for biodiesel production.

The thermodynamic properties are relevant for designing a batch-type reactor, essentially to determine the necessary volume and amount of heat transferred.

The global transesterification reaction to produce esters can involve three reversible consecutive alcoholysis reactions, as shown in Figure 6, for the reaction with methanol as the alcohol (A). In this reaction scheme, triglycerides (TG) are sequentially converted into diglycerides (DG), monoglycerides (MG) and glycerol (GL), and at each step, one mol of ester (E) is produced.

$$\mathrm{TG} + \mathrm{CH_3OH} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathrm{DG} + \mathrm{E}$$

$$\mathrm{DG} + \mathrm{CH_3OH} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} \mathrm{MG} + \mathrm{E}$$

$$\mathrm{MG} + \mathrm{CH_3OH} \underset{k_6}{\overset{k_5}{\rightleftharpoons}} \mathrm{GL} + \mathrm{E}$$

Figure 6. Consecutive alcoholysis

For each step, there are two rate constants. The global transesterification reaction, as shown in Figure 7, includes two rate constants, one for the forward reaction and one for the backward reaction.

$$\mathrm{TG} + 3\mathrm{CH_3OH} \underset{k_8}{\overset{k_7}{\rightleftharpoons}} \mathrm{GL} + 3\mathrm{E}$$

Figure 7. Global transesterification reaction

The fatty acid methyl ester (FAME) concentration in the mixture should be at least 96.5 wt.% to be considered biodiesel, according to ASTM D6751.

The rates of reaction can be described by Equations (5)-(10). Together, these power law rate equations describe the kinetic model of the conversion of vegetable oil into biodiesel.

$$\frac{d[TG]}{dt} = -k_1[TG][A] + k_2[DG][E] \tag{5}$$

$$\frac{d[DG]}{dt} = k_1[TG][A] - k_2[DG][E] - k_3[DG][A] + k_4[MG][E] \tag{6}$$

$$\frac{d[MG]}{dt} = k_3[DG][A] - k_4[MG][E] - k_5[MG][A] + k_6[GL][E] \tag{7}$$

$$\frac{d[E]}{dt} = k_1[TG][A] - k_2[DG][E] + k_3[DG][A] - k_4[MG][E] + k_5[MG][A] - k_6[GL][E] \tag{8}$$

$$\frac{d[A]}{dt} = -\frac{d[E]}{dt} \tag{9}$$

$$\frac{d[GL]}{dt} = k_5[MG][A] - k_6[GL][E] \tag{10}$$

where:

$k_1, k_2, k_3, k_4, k_5, k_6$ = rate constants for the reactions in Figure 6, L/mol/min.
t = independent variable, min.
$[i]$ = concentration of the corresponding component i, mol/L.

The corresponding values of the rate constants at 323.15 K with methanol as the alcohol are shown in Table 9 [19]. According to the values of the rate constants, the conversion of MG into GL and E is much faster than its reversible reaction. Likewise, for the global reaction shown in Figure 6, the conversion of TG is approximately 5 times faster than its reversible reaction.

Table 9. Rate constants at 323.15 K for the transesterification of soybean oil with methanol[19]

Rate constant	Value, L/mol/min
k_1	0.050
k_2	0.110
k_3	0.215
k_4	1.228
k_5	0.242
k_6	0.007
k_7	7.84E-5
k_8	1.58E-5

In our case study, the feed to the batch reactor consisted of 35 kg of soybean oil and methanol at a ratio of 6 mol alcohol/1 mol of oil. The reactor operates at a constant pressure of 1 bar. The size of the reactor required for such feedstock and the duty of the reactor are needed.

By running the program, the properties of the soybean oil are determined. The soybean oil composition in Table 1 was used as a basis to determine the composition in terms of the mol fraction. The molecular weight of soybean oil is 875.453, and that of biodiesel is 293.162. The free fatty acid concentration is assumed to be null, so the triglycerides and esters have the same value in composition. The molecular weights of both the soybean oil and its biodiesel were also determined.

By integrating the differential equation of a batch reactor, the concentrations of the compounds can be determined. Thus, the volume required for the reactor is 48.3 L.

The amount of heat that needs to be transferred (duty) in the reactor to keep the temperature constant can be determined via Equation (11), assuming that the nonideal liquid phase is negligible.

$$Q = V \Delta H_{rxn} r \qquad (11)$$

where:
V = 48.3 liters
ΔH_{rxn} = enthalpy of reaction at 323 K

The reaction rate (r) is given by Equation (12), which represents the kinetics of the global reaction.

$$r = -k_7[TG][A]^3 + K_8[GL][E]^3 \qquad (12)$$

The ΔH_{rxn} determined with the program is 599.69 KJ/mol. indicating that the transesterification reaction is endothermic. When Eq. (11) is solved, the duty is equal to -4.8 KJ/mol.

4. CONCLUSIONS

The software developed in this program has the advantage of allowing the user to assemble the molecule by adding functional groups that constitute the different compounds involved in biodiesel conversion. Upon completion, the user can visualize the molecule. This contributes to a better understanding of the chemistry of the biodiesel production process.

Software efficiency and optimization are relevant when a considerable number of floating-point operations are performed, especially when there are iterations where there is a risk of numerical error accumulation. This is not the case with this program because each detected group is processed independently, and its contributions to the thermodynamic properties are calculated only once. The implemented equations have fewer than 10 floating-point operations, so the precision of the 32-bit floating-point data type is considered sufficient. The results and visualization are obtained almost instantaneously, so there is no need to improve efficiency. An elaborate data model is not required because the compound descriptions are in text files that are not modified by the program, and no report file is generated.

The software helps the user better understand the thermochemistry and kinetics of the transesterification reactions that occur with different types of vegetable oil. Furthermore, the program can be applied to determine the heat of combustion and the amount of heat transferred, which is very useful for fuel optimization and reactor performance.

In future work, the program will be modified to include different types of reactors, including kinetic, thermodynamic, stoichiometric and yield reactors; in this way, we expect to extend the program into a biodiesel reactor simulator.

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