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Green fuel synthesis from Jatropha curcas seed oil: A Computational Approach using python programming language

Abstract: - The depletion of fossil fuels and environmental concerns in the recent era has gained significant attention in the production of biodiesel from non-edible seed oils as an alternative fuel. Biodiesel is one of the renewable fuel to replace fossil fuel. The synthesis of biodiesel from the seed oils is time consuming and costly. In order to predict new seed oils in biodiesel synthesis, several studies have been conducted to suggest the advantages of artificial intelligence in the field of producing green energy. The fourth industrial revolution is thought to be fuelled by artificial intelligence (AI) and machine learning algorithms, which can understand complicated issues with non-linear correlations. In the present study attempt has been made to predict the fuel properties of Jatropha curcas seed oil using python programming language. The fatty acid composition required for calculation is derived from literature. This code can be preserved and used multiple times to analyse the fuel properties which is time saving. The values obtained are well within the range of ASTM and EN standards.

Keywords: Biodiesel, Jatropha curcas, fuel properties, python, seed oil

1. Introduction

The dwindling supply of fossil fuels is a result of the current energy situation, where there is high demand in the industrial and transportation sectors. The development of renewable energy sources has been motivated by the depletion of petroleum reserves, rising oil prices, and greenhouse gas emissions [1]. The greatest alternative that can replace commercial petro-diesel without modifying engines is biodiesel, which burns cleaner than petrodiesel [2]. A mixture of mono alkyl esters of long chain fatty acids generated from vegetable oils or animal fats is referred to as biodiesel [3]. Vegetable oil cannot be used directly in IC engines due to its high viscosity, which results in poor atomization and high engine deposits [4]. There are several ways to deal with the viscosity issue, including mixing, micro-emulsification The effective and widely used process, known as transesterification, creates esters and glycerol when vegetable oil and alcohol react in the presence of a catalyst [5]. Glycerol has several industrial uses, particularly in the pharmaceutical and cosmetics industries. Vegetable oil use is extremely problematic

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because it competes with the food industry and raises the price of biodiesel, therefore, researchers are concentrating on non-edible seed oils as the feedstock for biodiesel synthesis.

The choice of raw material in biodiesel synthesis is also made based on the amount of oil present in the seeds, as well as its chemical composition, suitability, and physical characteristics. The areas also influence the choice of raw materials used to make biodiesel. Palm oil, rapeseed oil, and soybean oil are the three main sources for the manufacturing of biodiesel in Europe and tropical nations [6]. In the USA, soybean is a significant feedstock.

In order to choose the best production method for biodiesel for smooth, efficient, and simpler processing, it is important to understand the fundamental information regarding the physicochemical, chemical, and physical parameters such as% FFA content, free fatty acid content, total saturated fatty acids, and total unsaturated fatty acids [3].

An essential factor in choosing the most effective way to produce biodiesel is the fatty acid contour of seed oils. The fatty acid content in seed oil diverges from one province to another for the similar types of seed oil as seeds are controlled by the geographical conditions [6]. The generally available fatty acids in seed vegetable oils include palmitic with 16 carbons and stearic with 18 carbons. Other vegetable oils also contain lauric, myristic acid, palmitoleic, oleic, linoleic, linolenic, arachidic, behenic and lignoceric acid [15]. Predominantly, fuel properties of biodiesel are determined by unsaturation content of the fatty acids.

Always experimental evaluation of biodiesel properties can be an expensive and lengthy process. A computational method can be used to predict fuel properties using standard mathematical models developed. This is a new trend in evaluating raw materials based on component fatty acids [7]. A useful method is to study non-edible seed oils and screen them for biodiesel properties using well-founded mathematical models. This method reduces the cost of experiments and time invested on analysis. A number of research teams have attempted to create mathematical models for assessing the characteristics of biodiesel derived from seed oil using the percentage of free fatty acids. This study evaluates *Jatropha curcas* seed oil using the aforementioned mathematical models. The mathematical models used in this work are more reliable with the experimental values and thus have the smallest deviation. Additionally, it also helps in recognizing the eminence of seed oil based on the fatty acids and their percentage composition. Thus, it contributes to the expansion of new chances for feed stock convenience methods and their permutations and combinations, which result in the addition of new prospective feed stocks to the currently inadequate feedstock sources.

One of the suitable programming languages used in this study is Python. Python is a well-designed language that works well for programming in the real world. Python is a very advanced, dynamic, object-oriented, general-purpose programming language that makes use of an interpreter and can be applied to a widespread array of applications. Python was created to be simple to learn and use. In recent years, Python has gained a reputation as a relatively user- and beginner-friendly language [8].

Although it can be resolved by the conventional mathematical models, Python programming preserves the code and allows for the evaluation of some of the properties of seed oils such as molecular weight, iodine value, saponification value, and viscosity, flash point, cloud point, and pour point by addressing the fatty acid composition. By definition, scientific computing is the use of mathematics and computation to the problem-solving of intricate engineering and scientific problems. It includes employing computers rather than human brains to solve a problem [9]. Here, simulations, modeling, and data analysis can all be done on computers. In a variety of disciplines, including physics, chemistry, biology, and engineering, it aids in our

comprehension and prediction of the behaviour of complex systems [10].

Table 1. Computational investigation using mathematical models for screening of seed oils

Eq No.	Equation	Terms	Ref.
i.	**Molecular weight of seed oil:** $Mw_{jo} = 3\ (Mw_{if}) + 3\ (Mw_{gly}) - 3\ (Mw_{alc})$	M_{wif} = molecular weight of each fatty acid	[11]

ii.	$\text{Sap Value} = \sum \frac{56.03 \text{ x Aif}}{Mwif}$	A_{if} - % of component fatty acids Mw_{if} -molecular mass of each component	[12]
iii.	$\text{Iodine Value} = \sum \frac{253.81 \text{x Ndb x Aif}}{Mwi}$	Aif - % of component each fatty acids Ndb - double bonds Mwi - molecular mass of each component	
iv.	$CN_{mix} = \sum A_C \text{ x } CN_{IC}$	A_C is the percentage composition of individual fatty acid ester, CN_{IC} is cetane number of respective fatty acid ester	[3]
v.	HHV = 49.43 – (0.015 x IV) – (0.041 x SV)	IV is iodine value and SV is saponification value	[12]
vi.	$LHV = 0.0011\left(\frac{H}{O}\right)^3 - 0.0785\left(\frac{H}{O}\right)^2 + 2.0409\left(\frac{H}{O}\right) + 20.992 - 0.100\,Ndb$ $LHV = 0.0901\left(\frac{C}{O}\right)^3 - 0.3515\left(\frac{C}{O}\right)^2 + 4.200\left(\frac{C}{O}\right) + 21.066 - 0.100\ Ndb$	C- carbon atoms, H - hydrogen atoms, O - oxygen atoms Ndb- number of double bonds.	[13]
vii.	FP = 205.226 + 0.083Mp –1.727Ms –0.5717Mo – 0.3557Mu– 0.467Mln – 0.2287Me	Mp, Ms, Mo, Mu, Mln, Me are mass fraction of palmitic, stearic, oleic, linoleic, linolenic and erucic acids respectively.	[13]
viii.	CP = – 0.576 x U_{fame} + 48.3	U_{fame} is % of unsaturation in methyl esters.	
ix.	PP = – 0.626 x U_{fame} + 45.694	U_{fame} is % of unsaturation in methyl esters.	

Table 2. Component fatty acids (CFAs) in *Jatropha curcas* seed oil

Physicochemical properties of oil	*JCSO*
Molecular weight	998.1
Saponification Value (mg KOH/g of seed oil)	169.3
Iodine Value (g I_2/100 g of seed oil)	103.3

Table 3. Physico-chemical properties of *Jatropha curcas* seed oil

CFAs	N_C:N_{db}	Molecular formula	Fatty acid composition of *JCSO* [14]
Myristic acid	14:0	$C_{14}H_{28}O_2$	1.4
Palmitic acid	16:0	$C_{16}H_{32}O_2$	14.62
Palmitoleic acid	16:1	$C_{16}H_{32}O_2$	1.47

Stearic acid	18:0	$C_{18}H_{36}O_2$	7.36
Oleic acid	18:1	$C_{18}H_{14}O_2$	41.43
Linoleic acid	18:2	$C_{18}H_{32}O_2$	35.42
Linolenic acid	18:3	$C_{18}H_{32}O_2$	0.2
Arachidic	20:0		0.3
%TSFA	-		16.32
%TUSFA	-		85.8

Table 4. Comparison of properties of biodiesels empirically computed for JCME, with experimental values of JCME and PD

Fuel property	***JCME***	***JCME [14]***	**PD**
CN	56.96	55.43	42.0
HHV (MJ kg^{-1})	45.5	40.7	46.0
LHV (MJ kg^{-1})	33.58	NA	43.1
Flash point (^{0}C)	157.3	175.5	120
Cloud point (^{0}C)	-1.12	5.6	-8.1
Pour point (^{0}C)	-8.01	6.0	-15

2. Result and discussion

The data required for computing and analysing the biodiesel properties of seed oils of *Jatropha curcas* are derived from the literature. The details of component fatty acids (CFAs) are depicted in Table-2 and other analytical values of seed oils and properties of biodiesel are depicted in Table-3 and Table 4.

2.1 Molecular weight of oil

The molecular weight of oil can be determined using the equation 1 as shown in Table 1. Fig. 1 shows the Python code for calculating the molecular weight of oil. Using Python programming, the molecular weight of *JCSO* was determined to be 998.11, as shown in Table 3 and Fig 2.

2.2 Saponification value

The milligrams of KOH needed to saponify one gram of oil is known as the saponification value. It is possible to establish a correlation between a certain biodiesel's fatty acid makeup and its specific volatility. It is computed using equation no. 2, which is shown in Table no. 1. Fig.3 shows the Python code for calculating the oil's saponification value. Using Python code, the saponification value of *JCSO* was determined to be 169.32 mg KOH/g of oil, as shown in Fig 4.

2.3 Iodine value

IV is a critical measure for seed oils that determines their suitability for use in the biodiesel synthesis process. IV is the degree of unsaturation, or the grams of iodine consumed by 100 g of oil. The limit specified by EN 14214 states that the oil content should not exceed 120 g I2/100 g. It is evident from the formula and the code's output that *Jatropha curcas* seed oil has an iodine value of 103.35 g I2/100 g of oil, which is why biodiesel synthesis uses it so frequently. Figure 5 shows the Python code used to determine the iodine value of seed oil, and Figure 6 shows the resultant iodine value of the *JCSO*.

2.4 Cetane number

Cetane number is another significant fuel statistic that helps in prediction the ignition quality of fuel. It is the proportion of n-cetane by volume in a flammable combination of n-cetane and 1-methyl naphthalene whose ignition properties coincide with test diesel. Because biodiesels have a greater CN content than traditional petro-

diesel, they burn more efficiently. The degree of unsaturation and chain length have a major influence on the CN of fatty acids. It increases as the chain length increases and falls as the unsaturation level drops. The cetane number of *JCME*, 56.96, is determined using a Python method and equation 4, as shown in Table 1. Petro diesel has a cetane number of 42.0, which appears to be lower than the *JCME* shown in Table 4. Figure 7 shows the output of the python code used to calculate the cetane number of seed oil, and Figure 8 shows the cetane number of *JCSO*.

2.5 Higher heating value

The amount of heat released by a specific quantity (at initial temperature of 25°C) of fuel once it has burned and the products have returned to a temperature of 25°C is known as the higher heating value (also known as gross calorific value or gross energy) of a fuel. This value accounts for the latent heat of condensation of water vapour in the combustion products. It is well known that the refined vegetable oils used in iesel engines are made up of intricate chemical combinations containing methyl esters of fatty acids. It is computed using equation 5, which Table 1 illustrates. Fig. 9 shows the Python code at a higher heating value. Using a Python algorithm, the higher heating value of *JCME* was predicted to be 45.5 MJ kg-1, as shown in Fig 10.

2.6 Lower heating value

The amount of heat released by burning a given quantity of fuel (initially at 25 °C) and raising the temperature of the combustion products to 150 °C is known as the lower heating value, or net calorific value, of a fuel. This calculation is based on the assumption that the latent heat of condensation of water vapour in the reaction products is not recovered. It is computed using equation 6, which Table 1 illustrates. Fig. 11 shows the Python code for a lower heating value. Using Python code, the lower heating value of JCME was determined to be 37.197 MJ kg-1, as shown in Fig. 12.

2.7 Flash point

The temperature at which a specific organic compound releases enough vapour to ignite in air is known as its flash point. It is one of the main flammability indices used to assess a liquid's risk of fire and explosion. Lower danger of fuel storage and transportation is indicated by higher FP [16]. It is computed using equation 7, which is shown in Table 1. Figs. 13 and 14 show the Python code for the biodiesel flash point. Using Python code, the computed flash point of JCME is 157.3 ^{0}C, greater than the petro-diesel shown in Table 4 and illustrated in Fig 15. This shows that the biodiesel obtained from Jatropha is risk free to store when compared with petro-diesel.

2.8 Cloud point and pour point

The intermolecular forces and molecular packing of a substance determine its crystallization. The fatty acid composition of the feedstock used to produce biodiesel determines the cold flow characteristics of the product. Improved cold flow characteristics are a result of the oil's increased unsaturated fatty acid concentration. On the other hand, biodiesel with lower cold flow characteristics is revealed to have a larger value of saturated fatty acids [31]. Oils with a larger concentration of heavier fatty acids demonstrated the same effect as those with a higher content of saturated fatty acids, as the cold flow qualities are likewise dependent on the chain length of fatty acids. Equations 8 and 9, respectively, are used to compute the cloud point and pour point of JCME and are shown in Table 1. Figs. 16 and 17 show the Python code for the biodiesel cloud point and pour point. Using Python code, the cloud point and pour of JCME were determined to be -1.120 C and -8.010 C, respectively. Figs. 18 and 19 illustrate these results. Petro-diesel has favourable flow characteristics. PP is -15^{0}C and CP is -8.1^{0}C Table 4 shows these numbers.

```python
# formula for molecular weight of oil
def mol_weight ():
    x = list(map(float, input("Enter seperate values of molecular weight in sequence: ").split()))
    y = len(x)
    mw = 0
    mwg = 92.09382*3
    mwa = 32.04*3
    for i in x:
        mw += (3*i) + mwg - mwa
    return mw/y
```

Fig 1: Python code for determination of molecular weight of oil

```
>>> mol_weight()
Enter seperate values of molecular weight in sequence: 228.3 256.4 256.4 284.4 282.4 280.4 280.4 312.5
998.1114600000001
>>>
```

Fig 2: Output of molecular weight using python code

```
#formula for saponification value
def sap_value():
    ai = list(map(float, input("Enter seperate values of %' composition in sequence: ").split()))
    mwi = list(map(float, input("Enter seperate values of molecular mass in sequence: ").split()))
    total = 0
    for i in ai:
        for j in mwi:
            total += (56.03*i)/j
    return total
```

Fig 3: Python code for determination of Saponification value of oil

```
>>> sap_value()
Enter seperate values of %' composition in sequence: 1.4 14.62 1.47 7.36 41.43 35.42 0.2 0.3
Enter seperate values of molecular mass in sequence: 228.3 256.4 256.4 284.4 282.4 280.4 280.4 312.5
169.32815941810767
>>>
```

Fig 4: Output of saponification value using python code

```
component_percentages = []
molecular_masses = []
double_bonds = []
for acid in fatty_acids:
    component_percentages.append(float(input(f"Enter the % component (Ai) of {acid['name']}: ")))
    molecular_masses.append(acid["mwi"])
    double_bonds.append(acid["ndb"])
# Calculate the iodine value (IV) for the whole data
iodine_value = calculate_iodine_value(component_percentages, molecular_masses, double_bonds)

# Print the result
print("Iodine Value (IV) for the whole data:", iodine_value)
```

Fig 5: Python code for determination of Iodine value of oil

```
PROBLEMS  OUTPUT  DEBUG CONSOLE  TERMINAL

PS C:\Users\DELL> & "C:/Program Files/Python311/python.exe" "c:/Users/DELL/Desktop/Python Programs; 22142/Iodine Value.py"
Enter the % component (Ai) of Myristic Acid: 1.4
Enter the % component (Ai) of Palmitic Acid: 14.62
Enter the % component (Ai) of Stearic Acid: 7.36
Enter the % component (Ai) of Palmitoleic Acid: 1.47
Enter the % component (Ai) of Oleic Acid: 41.43
Enter the % component (Ai) of Linoleic Acid: 35.42
Enter the % component (Ai) of Linolenic Acid: 0.2
Enter the % component (Ai) of Arachidic Acid: 0.3
Iodine Value (IV) for the whole data: 103.35623294302464
PS C:\Users\DELL>
```

Fig 6: Output of Iodine value of oil using python code

```
def calculate_CNmix(compositions, cetane_numbers):
    if len(compositions) != len(cetane_numbers):
        raise ValueError("The number of compositions and cetane numbers must be equal.")
    CNmix = 0
    for i in range(len(compositions)):
        CNmix += (compositions[i]/100) * cetane_numbers[i]
    return CNmix
# Data for specific fatty acids
fatty_acids = [
    {"name": "Myristic Acid", "CN": 66.2},
    {"name": "Palmitic Acid", "CN": 74.5},
    {"name": "Stearic Acid", "CN": 86.9},
    {"name": "Palmitoleic Acid", "CN": 51},
    {"name": "Oleic Acid", "CN": 55},
    {"name": "Linoleic Acid", "CN": 42.2},
    {"name": "Linolenic Acid", "CN": 20.6},
    {"name": "Arachidic Acid", "CN": 74}
]
# Prompt the user to enter the composition (Ac) for each acid
compositions = []
cetane_numbers = []
for acid in fatty_acids:
    composition = float(input(f"Enter the composition (Ac) of {acid['name']}: "))
    compositions.append(composition)
    cetane_numbers.append(acid["CN"])
CNmix_value = calculate_CNmix(compositions, cetane_numbers)
print("CNmix value:", CNmix_value)
```

Fig 7: Python code for determination of cetane number of oil

```
PROBLEMS  OUTPUT  DEBUG CONSOLE  TERMINAL

PS C:\Users\DELL> & "C:/Program Files/Python311/python.exe" "c:/Users/DELL/Desktop/Python Programs; 22142/CNmix.py"
Enter the composition (Ac) of Myristic Acid: 1.4
Enter the composition (Ac) of Palmitic Acid: 14.62
Enter the composition (Ac) of Stearic Acid: 7.36
Enter the composition (Ac) of Palmitoleic Acid: 1.47
Enter the composition (Ac) of Oleic Acid: 41.43
Enter the composition (Ac) of Linoleic Acid: 35.42
Enter the composition (Ac) of Linolenic Acid: 0.2
Enter the composition (Ac) of Arachidic Acid: 0.3
CNmix value: 56.961180000000006
PS C:\Users\DELL>
```

Fig 8: Output of cetane number of oil using python code

```
#formula for higher heating value
def hhv():
    print("Please enter iodine value")
    iv = int(input())
    print("Please enter saponification value")
    sv = int(input())
    hhv = 49.43 - (0.015*iv) - (0.014*sv)
    return hhv
```

Fig 9: Python code for determination of Higher heating value

```
>>> hhv()
Please enter iodine value
103.5
Please enter saponification value
169.32
45.50702
>>>
```

Fig 10: Output of HHV of biodiesel using python code

```
#formula for lower heating value
def lhv():
    print("Please enter no. of carbon atoms")
    c = int(input())
    print("Please enter no. of hydrogen atoms")
    h = int(input())
    print("Please enter no. of oxygen atoms")
    o = int(input())
    print("Please enter no. of double bonds")
    ndb = int(input())
    lhv_1 = (0.0011*(h/o)**3) - (0.0785*(h/o)**2) + (2.0409*(h/o)) + (20.992) - (0.100*ndb)
    lhv_2 = (0.0901*(c/o)**3) - (0.3515*(c/o)**2) + (4.200*(c/o)) + (21.066) - (0.100*ndb)
    return lhv_1 , lhv_2
...
```

Fig 11: Python code for determination of Lower heating value

```
>>>
>>> lhv()
Please enter no. of carbon atoms
14
Please enter no. of hydrogen atoms
28
Please enter no. of oxygen atoms
2
Please enter no. of double bonds
0
(37.197, 64.1468)
>>>
```

Fig 12: Output of LHV of biodiesel using python cod

```
def calculate_flash_point(xp, xs, xo, xli, xln, xe):
    fp = 205.226 + 0.083 * xp - 1.727 * xs - 0.5717 * xo - 0.3557 * xli - 0.467 * xln - 0.2287 * xe
    return fp
```

Fig 13: Python code for determination of Flash point

```
def calculate_flash_point(xp, xs, xo, xli, xln, xe):
    fp = 205.226 + 0.083 * xp - 1.727 * xs - 0.5717 * xo - 0.3557 *
xli - 0.467 * xln - 0.2287 * xe
    return fp
# Prompt the user to enter the mass fractions of each fatty acid
while True:
    try:
        xp = float(input("Enter the mass fraction of Palmitic acid
(Xp): "))
        xs = float(input("Enter the mass fraction of Stearic acid
(Xs): "))
        xo = float(input("Enter the mass fraction of Oleic acid
(Xo): "))
        xli = float(input("Enter the mass fraction of Linoleic acid
(Xli): "))
        xln = float(input("Enter the mass fraction of Linolenic
acid (Xln): "))
        xe = float(input("Enter the mass fraction of Erucic acid
(Xe): "))
        break
    except ValueError:
        print("Invalid input. Please enter valid numerical
values.")
flash_point = calculate_flash_point(xp, xs, xo, xli, xln, xe)
print("Flash Point (FP):", flash_point ,"°C")
```

Fig 14 : Python code for determination of Flash point

```
PS C:\Users\DELL> & "C:/Program Files/Python311/python.exe" "c:/Users/DELL/Desktop/Python Programs; 22142/Flash point.py"
Enter the mass fraction of Palmitic acid (Xp): 14.62
Enter the mass fraction of Stearic acid (Xs): 7.36
Enter the mass fraction of Oleic acid (Xo): 41.43
Enter the mass fraction of Linoleic acid (Xli): 35.42
Enter the mass fraction of Linolenic acid (Xln): 0.2
Enter the mass fraction of Erucic acid (Xe): 0
Flash Point (FP): 157.350915 °C
PS C:\Users\DELL>
```

Fig 15: Output of Flash point value of oil using python code

3. Conclusion

The experimental procedures for biodiesel synthesis are time consuming and costs high. By using python coding, the oil properties and biodiesel properties of respective seed oils can be calculated. This helps in predicting the biodiesel fuel properties easily. This programming helps in preserving the codes and values. It also helps in predicting and analysing the fuel properties of new seeds selected for biodiesel synthesis in short time. The fuel properties of *Jatropha curcas* methyl esters calculated using python code meet the major specifications of US biodiesel standard and European standards and thus it's been utilized in the biodiesel production. The calculated values are obtained from the substantiated python model are similar to the values obtained from literature. This programming decreases experimental costs and investigation time of experimentation.

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