APPLICATION OF ASPEN HYSYS PROCESS SIMULATOR IN GREEN ENERGY REVOLUTION: A CASE STUDY OF BIODIESEL PRODUCTION

Abdulwahab Giwa¹, Saidat Olanipekun Giwa² and Ebenezer Ajibola Olugbade¹
¹Chemical and Petroleum Engineering Department, College of Engineering, Afe Babalola University, Afe Babalola Way, Ado-Ekiti, Ekiti State, Nigeria
²Chemical Engineering Department, Faculty of Engineering and Engineering Technology, Abubakar Tafawa Balewa University, Tafawa Balewa Way, Bauchi, Nigeria
Email: agiwa@abuad.edu.ng

ABSTRACT

Green economic revolution is a system that brings about improved human well-being and social equity while significantly reducing carbon emissions, enhancing energy efficiency and lessening environmental degradation. One of its sectors is renewable energy production, which is energy development from naturally replenished resources. Renewable energy types include solar power, wind power, hydroelectricity, biomass and biofuels. The most common biofuel is biodiesel, which can be produced from oils/fats using transesterification process or from fatty acids using esterification process. The process of biodiesel production can be simulated with the aid of a process simulator via either the conventional method of a reaction followed by separation or an integrated method known as reactive distillation. To demonstrate the simulation, this work has been carried out to achieve production of biodiesel for green economic revolution using the two methods with the aid of Aspen HYSYS process simulator. The performances of the two methods in biodiesel production were evaluated, and it was discovered that reactive distillation approach was more efficient and effective than the conventional one because more amount, and, of course, better purity, of biodiesel was given by the reactive distillation process compared to the conventional method. Thus, Aspen HYSYS has been successfully applied in analysing biodiesel production by the two methods to know which of the alternatives the best is effectively and efficiently. It is, therefore, recommended that scientists should apply the process simulator to study chemical reactions prior to any laboratory experiment.

Keywords: green economic revolution, biodiesel, conventional method, reactive distillation, Aspen HYSYS.

1. INTRODUCTION

Green economy is one that leads to improvement in the well-being and social equity of humans, while significantly reducing environmental risks and ecological scarcities. This economy is a model based on sustainable development and knowledge of ecological economics [1]. At present, Green economy can be said to be a substitute vision for growth and development; that is, one through which growth and improvements in people’s lives can be generated in ways that are reliable with sustainable development. A green economy involves a triple bottom line, viz. sustaining and advancing economics, environmental, and social wellbeing [1], and it is buttressed by three major pillars, which are (1) low-carbon technology (2) resource – use efficiency and (3) socially inclusive growth [2].

The severe poverty amid plenty as well as the extensive environmental degradation across all regions are linked to a high dependence on the exploitation of natural resources in inefficient ways for livelihood activities, and this reinforces the cycle of underdevelopment. With a shift to a green economy framework, tremendous opportunities that will bring out the benefits from rich natural resource endowments in pursuance of sustainable development would be provided [2].

The transition to a green economy, based on the concept of sustainable development, has been internationally recognized as a way of combining economic development, social welfare and environmental protection. The green economy is argued to lead to improved human well-being, social equity, as well as significantly reduced environmental risks [3, 5]. A green economy has an inner relationship with a clean energy policy and has a more politically applied focus [3]. The real value of environmental services and the real costs to the environment are included in national policies [3, 4]. As a practical matter, integrated green energy policies need, for being sustainable, to be founded both on energy diversification through the promotion of renewable energy (solar energy, wind energy, biomass energy or hybrid systems) and on energy management putting the accent on energy transport and distribution, energy savings, or thermal insulation and green buildings [6].

There is almost undisputed agreement that energy plays a pivotal role in national development. By and large, there is a high degree of relationship between energy use, economic growth, and level of development. The climate change due to greenhouse gas emissions and turbulence in oil and gas prices have turned global attention to green energy sources, which are environmentally friendly. The first sector of the green economy is renewable energy [4], and this has also been discovered to be the major components of the green energy sources [7, 8].

Renewable energy is a regenerative energy derived from sources that are not prone to depletion in the human time scale, and they include biomass, solar, hydro,
Biodiesel, as a renewable energy, is a fuel made from plant oils and can be used in diesel engines [9]. It can be directly used to replace petroleum diesel without modifying diesel engines because their properties are similar [10-16]. Also, it is a promising alternative to conventional petroleum-based diesel fuel, and it has a number of other benefits such as reducing carbon dioxide emissions by about 78%, nontoxicity and biodegradability. These benefits have made biodiesel a very good environmentally benign one. Furthermore, biodiesel has properties that are more superior to those of petro-diesel fuel such as nontoxicity. Researches involving the production of biodiesel are being embarked on nowadays because it is very important for today’s world to identify an alternative to fossil fuel to meet the future demands for energy while satisfying the concept of green economy based on the fact that diesel fossil fuel reserves are dwindling and, at a time, they may run out [15-17] especially for use in internal combustion engines [8].

Biodiesels have been discovered to be typically made from renewable organic raw materials such as jatropha, soybean or rapeseed oils, animal fats, waste vegetable oils or microalgal oils. Their production methods include direct use and blending, microemulsions, thermal cracking and esterification/transesterification.

Esterification/transesterification is the most popular method of biodiesel production, and in that method, fatty acids/vegetable oils and animal fats are used as feed stocks. The production of biodiesel using esterification/transesterification can, actually, be accomplished through either conventional method of a reactor followed by series of separation or reactive distillation [11, 13, 18].

The conventional method of biodiesel production is carried out by esterification or transesterification process in the presence of a catalyst using a stirred tank reactor followed by purification [19] while reactive distillation is a process that is capable of combining both separation and chemical reaction in a single equipment unit[20-23]. Reactive distillation has a lot of advantages especially for those reactions occurring at suitable and appropriate conditions for the distillation of the reaction components [11-12, 24-31]. Apart from that, this process combines the benefits of equilibrium reaction with distillation in order to achieve a substantial progress in promoting reaction conversion as a result of constant recycling of unconverted materials and removal of products. As such, the process is able to reduce capital and operating costs as a result of the reduction that occurs in the number of equipment units of the plant [11, 31-33]. In addition to the advantages mentioned before, basically, the combination of reaction and distillation in the same equipment unit gives rise to suppression of side reaction(s) and utilization of heat evolved from an exothermic reaction for mass transfer operation. These synergistic effects of the process result in low energy cost and high product yields [9, 31-34]. The accomplishment of this process can be achieved theoretically via the application of a process simulator like Aspen HYSYS.

Aspen HYSYS is a process simulation environment designed to serve many processing industries. It is an interactive, intuitive, open and extensible program. It also has many add-on options to extend its capabilities into specific industries. With this program, rigorous steady state and dynamic models for plant design can be created. Apart from that, monitoring, troubleshooting, operational improvement, business planning and asset management can be performed with the aid of the process simulator. Through its completely interactive interface, process variables and unit operation topology can be easily manipulated [35-36].

The information obtained from the literature has revealed that some researches have been carried out on the application of this process simulator (Aspen HYSYS) to production of biodiesel, which is a renewable energy type. For instance, West et al. [37] modelled and simulated four continuous biodiesel processes using Aspen HYSYS. The first two processes employed traditional homogeneous alkali and acid catalysts while the third and the fourth processes used a heterogeneous acid catalyst and a supercritical method, respectively, to convert a waste vegetable oil feedstock into biodiesel. Santana et al. [38] designed and simulated a continuous biodiesel plant using castor oil as feedstock with the aid of Aspen HYSYS simulator. Simasatitkul et al. [10] used Aspen HYSYS to investigate the production of biodiesel from the transesterification reaction between soybean oil and methanol in a reactive distillation column and analysed the effects of some operating and design parameters on biodiesel production. Lee et al. [39] simulated three continuous biodiesel processes with production capacity of 40,000 tonne/yr, including a conventionalkali-catalyzed process using both fresh and waste vegetable oil and a supercritical methanol process using waste vegetable oil as the raw material with the aid of Aspen HYSYS. Ravindra et al. [40] employed Aspen HYSYS to develop model for enzyme catalyzed and conventional alkali-catalyzed biodiesel production processes in order to investigate the environmental performance of the enzyme-catalyzed process in comparison with the conventional alkali-catalyzed one using life cycle analysis (LCA). Orifici et al. [41] used Aspen HYSYS to simulate and optimize the process of biodiesel production from the transesterification reaction of crude palm oil with methanol. Karacan and Karacan [42] employed Aspen HYSYS for the simulation of reactive distillation that was used for the production of a fatty acid methyl ester (a biodiesel) at optimum conditions. According to the work, canola oil and methanol were used as feedstocks while potassium hydroxide and potassium methoxide were used as different formulations of catalysts. Giwa et al. [43] investigated the performance of some fatty acids used for the production of fatty acid methyl ester in a reactive distillation column with the aid of Aspen HYSYS. Giwa et al. [12] also
developed a prototype reactive distillation process for biodiesel production from which the data used for artificial neural network modelling of the process were generated. Furthermore, Giwa et al. [44] used the combination of Aspen HYSYS and Minitab to carry out the production of palmitic acid methyl ester, which is also a biodiesel. Ibrahim and Maraire [45] also used Aspen HYSYS to carry out the production of biodiesel from waste cooking oil. Tuluc et al. [46] carried out simulation and optimisation study for biodiesel synthesis process based on rapeseed oil transesterification with methanol in homogeneous catalysis by performing all necessary calculations with Aspen HYSYS process simulator. Farrag et al. [47] used some optimal process conditions to develop an Aspen HYSYS rigorous model for biodiesel production. Abdurakhman et al. [26] used Aspen HYSYS to carry out the simulation of biodiesel production from waste cooking oil using membrane reactor and studying the effect of free fatty acid content and membrane separation effectiveness on biodiesel yield.

From the literature review, it has been discovered that no work has used Aspen HYSYS process simulator to carry out the simulation of biodiesel production comparing both the conventional and the reactive distillation processes. Therefore, this work is carried out to bridge this gap by applying Aspen HYSYS process simulator to biodiesel production using the method of reactor followed by separation and the integrated one involving the simultaneous occurrence of reaction and separation in a single unit.

2. METHODOLOGY

The approach used in carrying out this study is the application of Aspen HYSYS [48] process simulator to develop and simulate the models of biodiesel production process via the conventional and the integrated (reactive distillation) methods.

The model developed for the conventional method of biodiesel production process with the aid of Aspen HYSYS is given in Figure-1. As can be seen from the figure, the process had two equipment units - a reactor and a distillation column. Two feed streams (linoleic acid and methanol) entering the reactor at the same temperature and pressure of 25 °C and 1 atm, respectively. The flow rate of the linoleic acid was 50 mL/min while that of the methanol was 10 mL/min. The fluid package used for the simulation of the conventional process was UNIversal QUAsi Chemical model (UNIQUAC).

The reaction (Equation 1) occurring in the reactor was modelled as an equilibrium type, the basis of which was activity in vapour phase and the equilibrium constant of which was estimated using Gibbs Free Energy. Furthermore, the distillation column used to purify the bottom product having higher amount of methyl linoleate (the desired product) was modelled to have 30 stages with its feed entering at the 15th stage. The pressure of each of its condenser and the reboiler was set to be 1 atm. Also, the reflux ratio of the distillation operation was 3kmol/kmol and the reboiler duty was 0.7kJ/s.

\[
C_nH_{2n+1}O_2 + CH _3OH \leftrightarrow C_nH_{2n}O_2 + H_2O
\]  

(1)

For the reactive distillation, the developed model obtained with the aid of Aspen HYSYS is given in Figure-2. Just as in the case of the reactor of the conventional model of the process, this one also had two feed streams. The upper feed stream, which was linoleic acid, entered the reactive distillation column at a temperature of 350 °C and a pressure of 5 atm while the lower feed stream, which was methanol, was passed into the column at a temperature and a pressure of 150 °C and 1 atm respectively. The reactive distillation column also had 30 stages, and the upper and the lower feed streams entered at the 8th and the 19th stages respectively. Similarly, the pressures of the condenser and the reboiler of the reactive distillation was 1 atm.

Figure-1. Aspen HYSYS conventional biodiesel production process model.
The reaction given in Equation (1) was also occurring between the two feed stages of the column. Being a reactive distillation process, the developed Aspen HYSYS was simulated using Sparse Continuation Solver. For the purpose of comparison, the reflux ratio and the reboiler duty of the reactive distillation column were also made to be 3 kmol/kmol and 0.7 kJ/s, respectively while the fluid package was also selected to be UNIversal QUAsiChemical model (UNIQUAC).

3. RESULTS AND DISCUSSIONS

The results obtained from the simulation of the model developed with the aid of Aspen HYSYS simulator for the production of biodiesel for green energy revolution from the esterification reaction between linoleic acid and methanol showed that a reaction conversion of approximately 73% can be achieved in the reactor of the conventional process. The value of the conversion was found not to be bad for a system like this.

Apart from the reaction conversion that was considered as the result of the simulation, the balances around each equipment of the process were as well investigated to ascertain the proper working of the process simulator.

Given in Table-1 are the molar flowrates of the components involved in the reaction taking place in the conventional process. As can be seen from the table, only linoleic acid and methanol entered the reactor while the mixture coming out of the reactor was containing all the four components involved in the process, but at different molar flow rates. It was also discovered from the results given in Table 1 that the desired product of the reaction, which was methyl linoleate (biodiesel) had the highest molar flow rate as the liquid (bottom) product of the reaction. The component with the highest mole flow rate at the top of the reactor, which was coming out as vapour, was methanol. That methanol was, actually, the unreacted one of the process. It was also noticed from the results that the system was operating at steady state because the total molar flow rate of the input was equal to that of the output.

![Figure-2. Aspen HYSYS reactive distillation biodiesel production process model.](image-url)
Table-1. Molar flowrates of the components involved in the reaction of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>gmol/min</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Input</td>
<td>Output</td>
<td>Total</td>
<td>Linoleic acid</td>
<td>Methanol</td>
<td>Top product</td>
<td>Bottom product</td>
<td>Input</td>
<td>Output</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>0.1620</td>
<td>0.0044</td>
<td>0.0398</td>
<td>0.1620</td>
<td>0.0442</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>0.1284</td>
<td>0.0021</td>
<td>0.2483</td>
<td>0.1305</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0401</td>
<td>0.0777</td>
<td>0.0000</td>
<td>0.1178</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.1153</td>
<td>0.0025</td>
<td>0.0000</td>
<td>0.1178</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>0.1620</td>
<td>0.2883</td>
<td>0.1221</td>
<td>0.4104</td>
<td>0.4104</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table-2 gives the mass flow rates of the components involved in the reaction of the conventional process of biodiesel production for green energy revolution, which has been simulated with the aid of Aspen HYSYS process simulator. The observations made in the case of this mass flow rate of the components were found to be similar to those of the molar flow rates. For instance, in this case also, the total mass flow rates of both the input and the output of the reactor were approximately the same. This was another indication that the system was operating at steady state, and that the law of conservation of mass has been obeyed by the process simulator. In addition, the component with the highest mass flow rate in the liquid product of the reaction was discovered to be the desired product, which was methyl linoleate.

Table-2. Mass flowrates of the components involved in the reaction of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>g/min</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Input</td>
<td>Output</td>
<td>Total</td>
<td>Linoleic acid</td>
<td>Methanol</td>
<td>Top product</td>
<td>Bottom product</td>
<td>Input</td>
<td>Output</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>45.4391</td>
<td>1.2352</td>
<td>11.1599</td>
<td>45.4391</td>
<td>12.3951</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>4.1157</td>
<td>0.0662</td>
<td>7.9572</td>
<td>4.1819</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>11.8171</td>
<td>22.8774</td>
<td>0.0000</td>
<td>34.6945</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>2.0771</td>
<td>0.0455</td>
<td>0.0000</td>
<td>2.1226</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>45.4391</td>
<td>19.2451</td>
<td>34.1490</td>
<td>53.3963</td>
<td>53.3942</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Also, considered as the results of this work were the volume flow rates of the components involved in the reaction of the conventional process. In the case, the highest volume flow rate was observed to be possessed by methyl linoleate in the liquid product of the process reaction. Unreacted linoleic acid and methanol were found to dominate the vapour product volume of the reactor.

Table-3. Volume flow rates of the components involved in the reaction of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>mL/min</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Input</td>
<td>Output</td>
<td>Total</td>
<td>Linoleic acid</td>
<td>Methanol</td>
<td>Top product</td>
<td>Bottom product</td>
<td>Input</td>
<td>Output</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>50.0000</td>
<td>1.3592</td>
<td>12.2801</td>
<td>50.0000</td>
<td>13.6393</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>5.1723</td>
<td>0.0832</td>
<td>10.0000</td>
<td>5.2555</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>13.2986</td>
<td>25.7455</td>
<td>0.0000</td>
<td>39.0441</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>2.0813</td>
<td>0.0456</td>
<td>0.0000</td>
<td>2.1269</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>50.0000</td>
<td>21.9114</td>
<td>38.1543</td>
<td>60.0000</td>
<td>60.0657</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 4. Molar compositions of the components involved in the reaction of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>Input Molar fraction</th>
<th>Output Molar fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linoleic acid</td>
<td>1.0000</td>
<td>0.0153</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>0.3260</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0153</td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>0.3260</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
<td></td>
</tr>
</tbody>
</table>

Table 5. Mass compositions of the components involved in the reaction of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>Input Mass fraction</th>
<th>Output Mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linoleic acid</td>
<td>1.0000</td>
<td>0.0642</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0699</td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Table 6. Volume compositions of the components involved in the reaction of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>Input Volume fraction</th>
<th>Output Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linoleic acid</td>
<td>1.0000</td>
<td>0.0620</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0748</td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Given in Tables 4, 5 and 6 are respectively the molar, the mass and the volume compositions of the components involved in the reaction of the conventional process of the biodiesel production. As can be seen from the tables, based on the fact that biodiesel (methyl linoleate) was given from the bottom of the reactor, it was found to have the highest molar, mass and volume fractions as the liquid bottom product of the process whereas the unreacted methanol had the highest molar, mass and volume fractions in the vapour top product of the process.

Table 7. Molar flow rates of the components involved in the separation of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>gmol/min</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linoleic acid</td>
<td>0.0398</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0021</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0777</td>
</tr>
<tr>
<td>Water</td>
<td>0.0025</td>
</tr>
<tr>
<td>Total</td>
<td>0.1221</td>
</tr>
</tbody>
</table>
Owing to the fact that it was deemed necessary to purify the product given at the bottom of the reactor, in which the desired product was present in large amount, it (the liquid product) was passed into a distillation column so as to distil the mixture and obtain higher purity of the desired product (biodiesel), and the results of the distillation are given thus.

Table-8. Mass flowrates of the components involved in the separation of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>g/min</th>
<th>Input</th>
<th>Top product</th>
<th>Bottom product</th>
<th>Total input</th>
<th>Total output</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linoleic acid</td>
<td>11.1599</td>
<td>7.5167</td>
<td>3.6432</td>
<td>11.1599</td>
<td>11.1599</td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0662</td>
<td>0.0662</td>
<td>0.0000</td>
<td>0.0662</td>
<td>0.0662</td>
<td></td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>22.8774</td>
<td>22.8774</td>
<td>0.0000</td>
<td>22.8774</td>
<td>22.8774</td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>0.0455</td>
<td>0.0455</td>
<td>0.0000</td>
<td>0.0455</td>
<td>0.0455</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>34.1490</td>
<td>30.5058</td>
<td>3.6432</td>
<td>34.1490</td>
<td>34.1490</td>
<td></td>
</tr>
</tbody>
</table>

Table-9. Volume flowrates of the component mixtures involved in the separation.

<table>
<thead>
<tr>
<th>Component</th>
<th>mL/min</th>
<th>Input</th>
<th>Top product</th>
<th>Bottom product</th>
<th>Total input</th>
<th>Total output</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linoleic acid</td>
<td>12.2801</td>
<td>8.2712</td>
<td>4.0089</td>
<td>12.2801</td>
<td>12.2801</td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0832</td>
<td>0.0832</td>
<td>0.0000</td>
<td>0.0832</td>
<td>0.0832</td>
<td></td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>25.7455</td>
<td>25.7455</td>
<td>0.0000</td>
<td>25.7455</td>
<td>25.7455</td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>0.0456</td>
<td>0.0456</td>
<td>0.0000</td>
<td>0.0456</td>
<td>0.0456</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>38.1543</td>
<td>34.1454</td>
<td>4.0089</td>
<td>38.1543</td>
<td>38.1543</td>
<td></td>
</tr>
</tbody>
</table>

Tables 7, 8 and 9 respectively give the molar, the mass and the volume flow rates of the components involved in the distillation operation of the conventional process of biodiesel production for green energy revolution. It was noticed from the results given in Tables 7-9 that the desired product, which was methyl linoleate, was coming from the top section of the column as a condensed liquid. According to the tables, the distillation operation was also found to occur at steady state because the total molar, the total mass and the total volume flow rates of the components in the input and the output of the distillation column were found to be approximately the same. This was also another point showing that the process simulator was obeying the law of conservation of mass, and this was observed to be an indication that the process simulator was functioning correctly.

Table-10. Molar compositions of the components involved in the separation of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>Molar fraction</th>
<th>Input</th>
<th>Top product</th>
<th>Bottom product</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linoleic acid</td>
<td>0.3260</td>
<td>0.2457</td>
<td>1.0000</td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0169</td>
<td>0.0189</td>
<td>0.0000</td>
<td></td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.6364</td>
<td>0.7122</td>
<td>0.0000</td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>0.0207</td>
<td>0.0232</td>
<td>0.0000</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td></td>
</tr>
</tbody>
</table>
Table-11. Mass compositions of the components involved in the separation of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>Mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Input</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>0.3268</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0019</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.6699</td>
</tr>
<tr>
<td>Water</td>
<td>0.0013</td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Table-12. Volume compositions of the components involved in the separation of the conventional process.

<table>
<thead>
<tr>
<th>Component</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Input</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>0.3219</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0022</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.6748</td>
</tr>
<tr>
<td>Water</td>
<td>0.0012</td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

The compositions of the components entering and leaving the distillation (separation) column of the conventional process of the biodiesel production revealed that the aim of the separation was achieved because, comparing the mole fraction, the mass fraction and the volume fraction of methyl linoleate entering the column, an improvement was seen as there was an increase in the compositions between the input and the output streams of the distillation column. The improvement in the compositions of the streams leaving the distillation column as compared to the one entering it was an indication that separation actually took place effectively.

Now, considering the results obtained from the reactive distillation process of the production of biodiesel, it can be noticed from Figure-3 showing the conversion profile of the column that, it was possible to achieve a conversion of more than 90% within the column. Comparing this conversion with the one obtained from the conventional production method, it was observed that higher conversion could be achieved in the reactive distillation column than that obtainable in the reactor of the conventional process alone. It can also be seen from Figure-3 that the reaction conversion decreased down the column towards the reboiler. It means that, for the production of biodiesel with very high conversion, the reaction should be made to occur at the stages of the reaction close to the upper feed stream.
Figure-3. Conversion profile of the reactive distillation process.

Table-13. Molar flowrates of the components involved in the reactive distillation.

<table>
<thead>
<tr>
<th>Component</th>
<th>gmol/min</th>
<th>Input</th>
<th>Output</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Linoleic acid</td>
<td>Methanol</td>
<td>Top product</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>0.3240</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.3240</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>0.6208</td>
<td>0.2840</td>
<td>0.0129</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.3240</td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.3097</td>
<td>0.0143</td>
</tr>
<tr>
<td>Total</td>
<td>0.3240</td>
<td>0.6208</td>
<td>0.5937</td>
<td>0.3512</td>
</tr>
</tbody>
</table>

Given in Table-13 is the molar flow rates of the components involved in the reactive distillation process of the biodiesel production for green energy revolution. As shown in the table, it was noticed that the system, in this case also, was operating at steady state because the total molar flow rates of both the input and that of the output were the same, despite the differences in the molar flow rates of the components. It should be noted that the differences in the molar flow rates of the components were due to the reaction (consumption and generation) occurring in the reaction (middle) section of the column.

Table-14. Mass flowrates of the components involved in the reactive distillation.

<table>
<thead>
<tr>
<th>Component</th>
<th>g/min</th>
<th>Input</th>
<th>Output</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Linoleic acid</td>
<td>Methanol</td>
<td>Top product</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>90.8781</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0111</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>19.8930</td>
<td>9.0989</td>
<td>0.4124</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0000</td>
<td>5.5801</td>
<td>0.2569</td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.0000</td>
<td>14.6790</td>
<td>96.0863</td>
</tr>
</tbody>
</table>
Table-15. Volume flowrates of the components involved in the reactive distillation.

<table>
<thead>
<tr>
<th>Component</th>
<th>mL/min</th>
<th>Input</th>
<th>Output</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Linoleic acid</td>
<td>Methanol</td>
<td>Top product</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>100.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0122</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>25.0000</td>
<td>11.4348</td>
<td>0.5183</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>107.3667</td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.0000</td>
<td>5.5914</td>
<td>0.2574</td>
</tr>
<tr>
<td>Total</td>
<td>100.0000</td>
<td>25.0000</td>
<td>17.0262</td>
<td>108.1546</td>
</tr>
</tbody>
</table>

The observations made for the mass (Table-14) and the volume (Table-15) flow rates of the components involved in the reactive distillation process were found to be similar to those of the molar flow rates because, although the values for components were not the same, they were found to be approximately the same for both the total input and the total output of the process.

Table-16. Molar compositions of the components involved in the reactive distillation.

<table>
<thead>
<tr>
<th>Component</th>
<th>Molar fraction</th>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Linoleic acid</td>
<td>Methanol</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>1.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>1.0000</td>
<td>0.4783</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.5217</td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Table-17. Mass compositions of the components involved in the reactive distillation.

<table>
<thead>
<tr>
<th>Component</th>
<th>Mass fraction</th>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Linoleic acid</td>
<td>Methanol</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>1.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>1.0000</td>
<td>0.6199</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.3801</td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Table-18. Volume compositions of the components involved in the reactive distillation.

<table>
<thead>
<tr>
<th>Component</th>
<th>Volume fraction</th>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Linoleic acid</td>
<td>Methanol</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>1.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0000</td>
<td>1.0000</td>
<td>0.6716</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>Water</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.3284</td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
The molar fractions, the mass fractions and the volume fractions of the components involved in the reactive distillation process of the production were also given in Tables 16, 17 and 18 respectively. Based on the results given in the tables, the desired product, which was methyl linoleate, had the highest mole, mass and volume fractions among all the components involved in the process.

Table 19. Comparison of molar fractions of the final products obtained from the two processes.

<table>
<thead>
<tr>
<th>Component</th>
<th>Conventional distillation</th>
<th>Reactive distillation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Top product</td>
<td>Bottom product</td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>0.2457</td>
<td>1.0000</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0189</td>
<td>0.0000</td>
</tr>
<tr>
<td>Methyl linoleate</td>
<td>0.7122</td>
<td>0.0000</td>
</tr>
<tr>
<td>Water</td>
<td>0.0232</td>
<td>0.0000</td>
</tr>
<tr>
<td>Total</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Moreover, finding out the better one between the two processes, a comparison was made between the molar fractions of the components obtained from both the conventional and the reactive distillation processes, and given in Table 19 are the results of the comparison. According to the table, the molar fraction of methyl linoleate obtained from the conventional process of biodiesel production was found to be less than that obtained from the reactive distillation process.

4. CONCLUSIONS

It has been revealed in this work that the production biodiesel, as a renewable energy source, which is also an energy source contributing to green energy revolution, can be simulated with the aid of Aspen HYSYS before carrying out the real experiment of it in the laboratory. It has also been shown that the use of reactive distillation for the production of biodiesel is more advantageous than the conventional method because more amount, and, of course, better purity, of biodiesel was given by the reactive distillation process.

ACKNOWLEDGEMENT

Special thanks go to Aare Afe Babalola, LL.B, FFPA, FNIALS, FCIArb, LL.D, SAN, OFR, CON - The Founder and President, and the Management of Afe Babalola University, Ado-Ekiti, Ekiti State, Nigeria for providing the necessary materials that enabled the accomplishment of this research work.

REFERENCES


[48] Aspen 2015. Aspen HYSYS V8.8 [34.0.0.8909], Aspen Technology, USA.