Process Simulation of Biodiesel Production from Soybean Oil with Aspen HYSYS: A Comparative Study of two different processes

S. Rafieyan [1], A. Bayat [2*]
[1] *Biomedical Engineering Department, Faculty of Chemical Engineering, Tarbiat Modares University, Tehran, Iran*
[2] *Department of Chemical Engineering, Tafresh University, Tafresh, 39518 79611 Iran*
bayat@tafreshu.ac.ir

Abstract
Biodiesel is one of the most promising green fuels at present which can be easily obtained from various vegetable oils/animal fats and even waste cooking oils. In recent years, researchers have investigated a lot about biodiesel production processes. In order to produce biodiesel in an industrial scale and optimize the process, it's needed firstly to simulate the production process to obtain information consistent with real data. In this respect, the vegetable oil fatty acid components (as a feedstock) were defined in detail. Afterward, two different processes suggested in the literature for biodiesel production were compared in terms of resource consumption and biodiesel yield.

Keywords: Biodiesel, Soybean Oil, Simulation, Aspen HYSYS

Introduction
Due to global warming as well as environmental issues caused by the use of fossil fuels, decrease in oil reserves and rising prices of crude oil, much attention has been devoted to renewable energies such as biofuels. One of the most promising biofuels is biodiesel [1, 2]. Biodiesel is a viable alternative to fossil fuels, and over the past several decades there has been a great deal of research on its production and improvement processes. Biodiesel can be produced from conventional transesterification of various sources such as vegetable oils, animal fats, microbial oils and waste cooking oil feedstocks [3, 4]. Transesterification reaction results in the conversion of Triglycerides (TG) to fatty acid methyl ester (FAME) which is called biodiesel. As can be seen in Fig. 1, TG reacts with a short chain alcohol in the presence of a catalyst to produce FAMEs and glycerol [5].

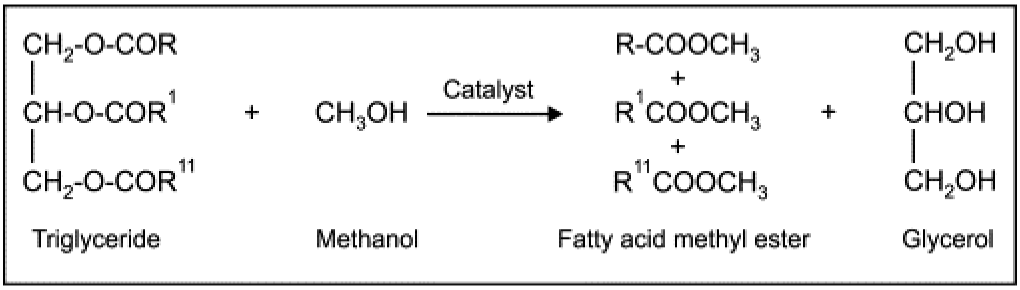


Figure 1 Transesterification reaction

Based on the reaction stoichiometry, the alcohol-to-oil ratio is 3: 1. However, excess alcohol is usually used to complete and shift the reaction towards the right side. Glycerol is produced as a by-product of transesterification of vegetable oils and animal fats. Therefore, after the reaction is complete, excess methanol and glycerol should be removed from reaction mixture [6, 7]. According to the ASTM D6751 (American Society for Testing and Materials), the amount of Methanol in the finished product should be less than 0.2% volumetric and the glycerol content should not exceed 0.24 wt.% [6].

One of the most common assumptions in the simulation of biodiesel production from vegetable oils is the use of only one fatty acid as a representative oil feedstock. Many researchers consider the fatty acid which has the highest percentage of the oil composition as a representative feedstock. However, in practice, each vegetable oil is made up of a combination of various fatty acids. So, in order to get closer to the actual results, it’s needed to consider the actual composition of the input feed as far as possible.

Zhang et al.[8] and Mello et al.[9] have introduced two different processes of biodiesel production as illustrated in Figure 2 and 3, respectively. Zhang utilized canola oil as feedstock to simulate the biodiesel production process and employed triolein as a representative of canola oil in the simulation. Methyl oleate was considered as the reaction product. On the other hand, Mello et al. applied soybean oil to produce biodiesel in the process simulation. According to Lawson [10], most of the soybean oil is consisted of linoleic acid. However, instead of considering just trilinoleic as a representative of soybean oil, a combination of five TGs as constituents of soybean oil was defined in the biodiesel simulation process.

In this study, the yields of biodiesel produced from soybean oil in both processes are compared while considering similar solvent, catalyst, conversion rate and production capacity. Instead of simplifying the simulation and using one fatty acid as a representative of all the fatty acids present in soybean oil, the detailed composition of several fatty acids that have the major portion in soybean oil has been considered and defined as feed in the simulation.

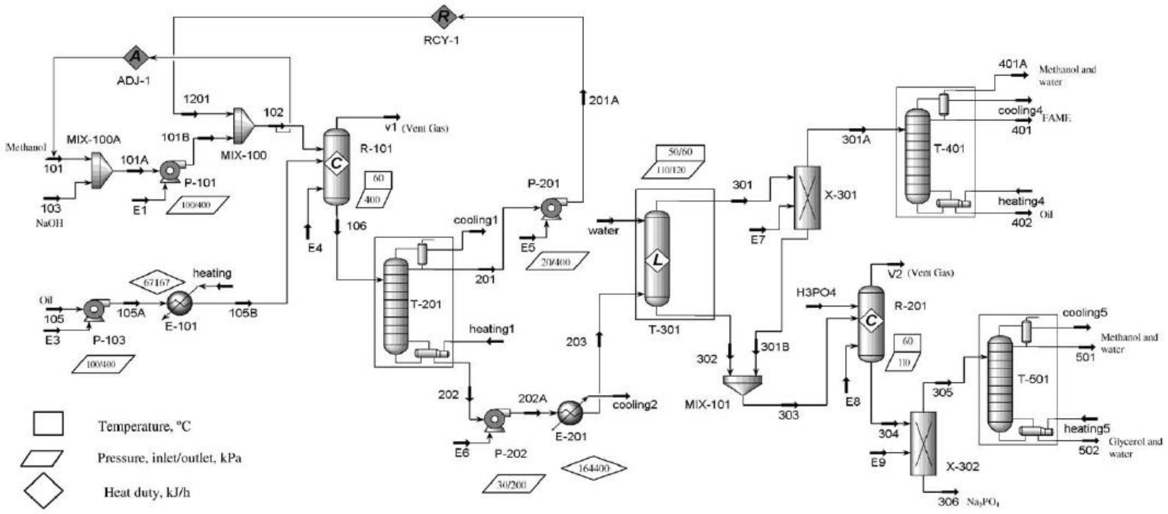


Figure 1 The process suggested by Zhang et al.

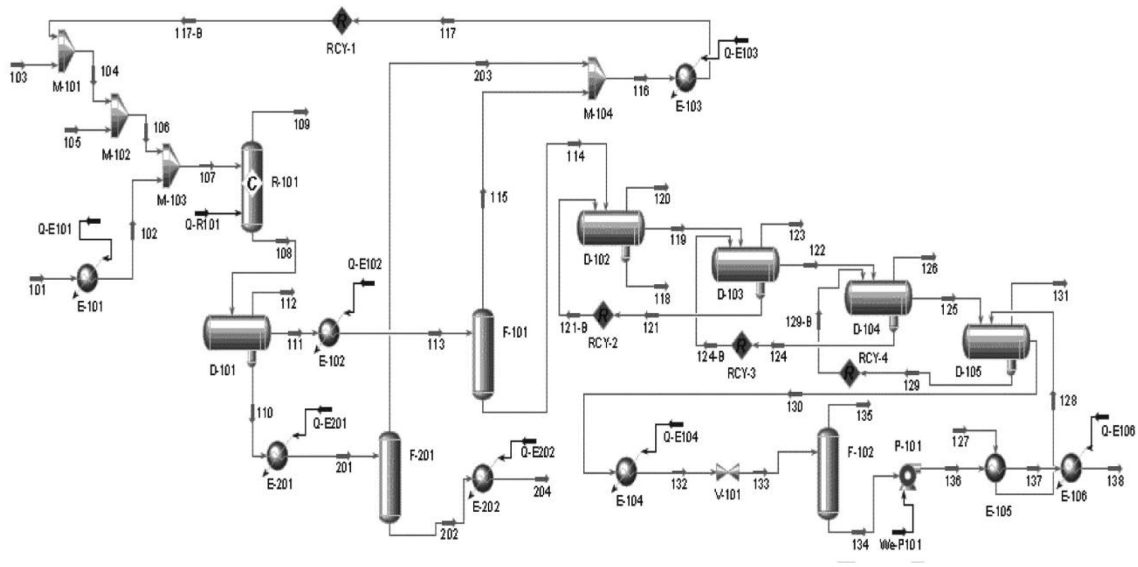


Figure 2 The process suggested by Mello et al.

Methods

Both processes for biodiesel production were simulated based on the data in the literature (According to information provided by Mello et al.) for a capacity of 7920 tons per year (Assuming operation duration as 24 hours a day and 330 days in a year). Aspen HYSYS (Version 10, Aspen Tech Inc.) was employed for the simulation of the aforesaid biodiesel production processes. The steps to perform the simulation include selecting the chemical components and thermodynamic fluid package, defining reactions and specifying operating conditions, consecutively. Aspen HYSYS includes most of the components such as methanol, glycerol, sodium hydroxide, and water which are required to simulate the processes in the databank library. However, some fatty acids of soybean oil which are not present in the databank should be defined as hypothetical components.

In many studies, NRTL (non-random two-liquid) and UNIQUAC (universal quasichemical) were selected as the thermodynamic fluid package. Thus, in this contribution, UNIQUAC

thermodynamic model was employed to predict the properties. The chemical reactions were defined based on the stoichiometry as illustrated in Figure 1, and the conversion rate was considered as 98%.
The operating conditions of each process (temperature, pressure, flow rate and composition of each stream) were specified in Aspen HYSYS as described in the corresponding process flow diagrams (PFDs). The reaction was performed under atmospheric pressure. The reaction temperature was considered at 60 °C. To ensure complete transesterification reaction, the molar ratio of methanol to vegetable oil was adjusted at 6:1 and the catalyst content was 1% wt. of vegetable oil.

Results and discussion

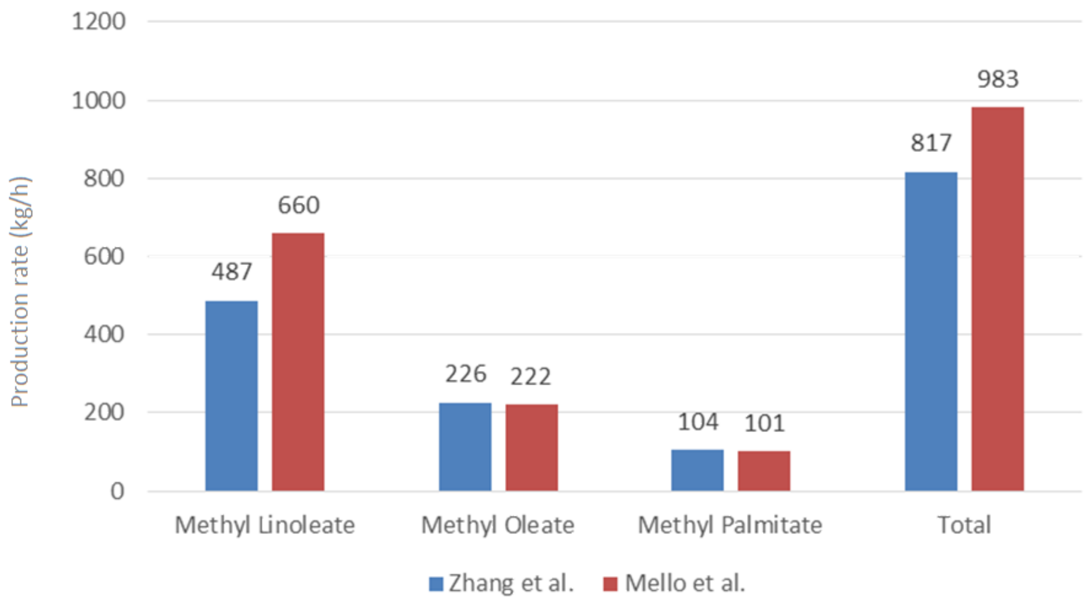
Using a precise composition of soybean oil in this simulation allowed us to better simulate the actual conditions. Accordingly, the detailed information of soybean oil from Mello et al. was utilized. These data were used to re-simulate and compare both suggested processes.
Some important input data of the simulation were provided in Table 1. Both processes were simulated with similar feed specifications. The final output data of the simulation cases were given in Table 2. As can be seen in the table, at the same feed capacity, the process provided by Mello et al. required about 99.2% more water (11880 ton/year compared to 87.12 ton/year) for water washing section while produced 17% more biodiesel (7786 ton/year compare to 6466 ton/year). The lower amount of biodiesel produced using the process suggested by Zhang et al. may be due to the loss of efficient water washing and biodiesel separation from the other components in the final stage. On the other hand, the enormous amount of water required in the process of Mello, with similar feed flow rate and little difference in the amount of final product composition, should be economically justified. As mentioned earlier, according to the standard, the amount of methanol and glycerol in the output product should be less than 0.2 %v. and 0.24 %wt., respectively. As depicted in Table 2, in both processes, these mentioned conditions are approximately met.
The major components of soybean biodiesel are depicted in Figure 4. According to the figure, as expected, the main component of biodiesel produced in both processes was Methyl Linoleate. The reason may be due to high amount of this fatty acid in the structure of the soybean oil (more than 50%)

Table 1. Input stream data of both process schemes

	Zhang et al.	Mello et al.	Unit
Soybean Oil (Feed)	7920	7920	ton/year
Methanol	930	930	ton/year
NaOH	79.2	79.2	ton/year
Reactor conversion	98	98	percentage

Table 2. Some important data of final product streams

	Zhang et al.	Mello et al.	Unit
biodiesel production	6466	7786	ton/year
Water Consumption	87.12	11880	ton/year
Methanol	0.27	0.22	m^3/year
Glycerol	0	0.09	percentage



.

Figure 4. Major Components of Soybean Biodiesel

Conclusions

According to input data retrieved from the literature, two processes for biodiesel production from soybean oil were simulated and the output results were compared. The process suggested by Zhang et al. consumed lower amount of water. Furthermore, the amount of glycerol present in the final biodiesel product was lower. On the other hand, the process suggedted by Mello et al. yielded higher amount of biodiesel. It should be noted that, thorough understanding and selecting the best process needs techno-economic investigation of the processes which is under way.

Acknowledgements

We gratefully acknowledge Mr. Farshad Golshan from BASF for his helpful comments in simulating the process.

References

[1] De R, Bhartiya S. and Shastri Y.," Multi-objective optimization of integrated biodiesel production and separation system", Fuel., 243, 519-532 (2019).

[2] Abbaszaadeh, A., Ghobadian, B., Omidkhah, M. R. and Najafi G.," Current biodiesel production technologies: A comparative review", Energy Conversion and Management., 63, 138-148 (2012).

[3] Baêsso, R. M., Costa Felix, R. P. B., Miloro, P. and Zeqiri B.," Ultrasonic parameter measurement as a means of assessing the quality of biodiesel production", Fuel., 241, 155-163 (2019).

[4] Chebbi, H., Leiva Candia, D., Carmona Cabello M., Jaouani, A., Dorado, M. P.," Biodiesel production from microbial oil provided by oleaginous yeasts from olive oil mill wastewater growing on industrial glycerol", Industrial Crops and Products., 139, 111535 (2019).

[5] West AH, Posarac D. and Ellis N.," Assessment of four biodiesel production processes using HYSYS. Plant", Bioresource technology., 99, 14, 6587-6601 (2008).

[6] Chilev, C., Simeonov, E.," Simulation of biodiesel production by transesterification of vegetable oils", Journal of Chemical Technology and Metallurgy., 49, 5, 479-486 (2014).

[7] Santana, G. C. S, Martins, P. F., de Lima da Silva, N., Batistella, C.B., Maciel Filho, R. and Wolf Maciel M. R.," Simulation and cost estimate for biodiesel production using castor oil", Chemical Engineering Research and Design, 88, 5, 626-632 (2010).

[8] Zhang, Y., Dubé, M. A., McLean, D. D. and Kates, M.," Biodiesel production from waste cooking oil: 1. Process design and technological assessment", Bioresource technology., 89, 1, 1-16 (2003).

[9] de Mello, M., Young, A., Villardi, H., Pessoa, F. and Salgado A.," Biodiesel production by the methylic-alkaline and ethylic-enzymatic routes: Discussion of some environmental aspects", Journal of Cleaner Production., 144, 347-357 (2017).

[10] Lawson, H., The Basic Chemistry of Oils and Fats. Food Oils and Fats: Technology, Utilization, and Nutrition. Boston, MA: Springer US, 3-14 (1995).