



Steady-State Simulation and Economic Analysis of Methanol-to-Butene Process Using Aspen HYSYS

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Abstract The steady-state modelling and simulation as well as economic analysis of methanol-to-butene process have been carried out in this work. The methanol-to-butene process model was developed with the aid of Aspen HYSYS by selecting the components involved, the fluid package, which was Peng-Robinson Stryjek-Vera equation of state, and the pieces of process equipment involved. Also, the material and energy streams of the process were picked from the palette and attached to the flowsheet in Aspen HYSYS environment. The feed conditions and other parameters were inputted into the process model while being simulated to steady-state convergence. From the results obtained, it was discovered that the production of butene could be achieved successfully because the mole fraction of butene coming out of the plug flow reactor and the separator were found to be 0.3329 and 0.8424, respectively. Apart from that, the specifications carried out on the pieces of equipment used in the process to obtain the specified mole fraction of the butene from methanol indicated that the process could be easily set up as the dimensions estimated were good and moderate. Finally, the value of the rate of return of 20% obtained from the economic analysis carried out revealed the economically viability of the process.

Keywords Methanol, butene, modelling, simulation, Aspen HYSYS

1. Introduction

The main aim of process engineers is to convert raw materials into useful products. Methanol, being the raw material in this case, is sometimes referred to as wood alcohol because it was first produced as a by-product of charcoal manufacturing by destructive distillation of wood. However, almost all the methanol produced today is synthesized from hydrogen and carbon monoxide. This research is indirectly focused on using methanol as a raw material to produce hydrocarbons [1].

Here comes the big question that should interest the reader, which is “why is methanol used in the production of hydrocarbons?” Before answering this question, it is known that for humankind to continue existing, the basics or essentials such as food, clean water, shelter and clothing materials as well as large amounts of energy are required. Ever since the time where cavemen were able to find materials that could ignite fire, our ancestors have been using this idea for heating and cooking in order to live a less struggling life. Then the idea of wood and vegetation followed by peat moss arriving as a source of energy, but since the industrial revolution started, the major source of energy used was coal until oil and natural gas were discovered from fossil fuels formed by decayed organisms present underground under high pressure and temperature, as a better source of energy during the twentieth century. Since then, it has been known widely as a fact that hydrocarbons in which most of them are used as fuels for heating, propulsion, and electrical power generation are mostly obtained from fossil fuels such as petroleum oil and natural gas and, so, when most people think of hydrocarbons, they think of fossil fuels as the source, most especially petroleum products [1].



Responding to the question above, methanol is used as a raw material in this case because it is cheap and can be synthesized easily from natural gas. It has been discovered over the years that fossil fuels once combusted are not renewable or cannot be reused by humans as a source of energy. This means once it is consumed, it is consumed and there is no going back to its original form. The desire and hunger for this source of energy has caused the depletion of fossil fuels over time. The rate at which fossil fuels are consumed is more than the rate at which they are generated underground by nature. This now leads to the fossil fuels depleting with time from the principle of material balance [1].

Furthermore, our readily accessible oil and gas reserves may not last much past the twenty-first century, while coal reserve may be available for another century or two [2]. This implies that there is need to search for new ways and resources for the future to keep the world moving energetically. It is the search for the new ways that resulted in using methanol as a raw material to produce hydrocarbons. With the advent of this idea, the dependence of mankind dependence on crude oil and natural gas resources will diminish [1].

The production of methanol directly from still-available fossil fuel sources and the recycling of carbon dioxide via hydrogenative reductions are feasible and convenient ways to store energy generated from all possible sources including, alternative energy sources (solar, hydro, wind, geothermal, etc.) and atomic energy. In the short term, new efficient production of methanol not only from still-available natural gas sources (without going through the synthetic (syn) gas route) but also by the hydrogenative conversion of carbon dioxide from industrial exhausts, offers feasible new routes [2]. The methanol produced via these routes can be converted to hydrocarbons to obtain more useful products. The process of converting methanol to hydrocarbon was first discovered at Mobil, now ExxonMobil, in 1977, and it was designed with the aim of transforming methanol to products such as olefins and gasoline [1].

When a process is confirmed feasible by experiments in the laboratory, the task of producing it commercially is a challenge that invites the expertise of process engineers. In chemical engineering, the process of converting from laboratory scale to industrial or commercial scale is known as a scale-up process. This means the chemical engineer's job in this case is to scale up the production of hydrocarbons from methanol in the laboratory to an industrial scale. That sounds easy but as easy as it may seem, the chemical engineer will need to perform tedious computations in order to achieve this goal. These days, computers are now employed in performing these tedious computations [1] through the use of process simulators, one of which is Aspen HYSYS.

Aspen HYSYS is a process simulator widely used at industrial level, especially in conceptual design and detailed engineering, control, optimization and process monitoring stages of a project. The most important applications of Aspen HYSYS correspond to the industries of oil and gas processing, refineries, and some industries of air separation. All these practices take advantage of this simulator architecture that permits the integration of steady-state and dynamic models. In this way, it is possible to bring together the stages of process design with the rigorous analysis of the dynamic behaviour and the control of the same to evaluate, in a direct way, the effects that the decisions in the detailed design step have over the dynamic and controllability of the process [3].

Reviewing information obtained from literature, similar researches relating to the subject matter are outlined thus. Hadi *et al.* [4] carried out series of experiments where methanol and water were mixed as feed for the methanol to propylene (MTP) process in temperature range of 623-823 K. According to this source, the H-ZSM5 catalyst with the Si/Al ratio of 200 was applied for carrying out the experiments. Also, a novel lumped kinetic model was proposed for methanol-to-propylene (MTP) process. The reactor was mathematically modelled by assumptions of being isothermal, fixed bed, plug flow and hybrid genetic algorithm was applied for estimating the kinetic parameters. A good agreement was observed between the experimental and the calculation data. The effect of temperature on propylene and ethylene sensitivity was investigated, and it was found that the propylene selectivity increased with temperature until 773.15 K, after which it decreased. Bos *et al.* [5] developed a kinetic model for methanol-to-olefin (MTO) process based on SAPO-34 molecular sieve. The final scheme they used consisted of 12 reactions involving 6 product lumps plus coke. Gayubo *et al.* [6] also proposed another kinetic model for the MTO process on the same SAPO-34. The kinetic parameters of this model were obtained by experiments that were carried out in a fixed bed isothermal reactor. Hadi *et al.* [7] suggested a kinetic model for the methanol-to-propylene (MTP) on Mn/H-ZSM5 catalyst based on the theory of



hydrocarbon pool and conjugate methylation or cracking reactions using a fixed bed reactor. The kinetic model consisted of 17 reactions and 14 chemical species in which methanol dehydrated to form olefins. Wu *et al.* [8] proposed a kinetic model for the MTP process over a high silica H-ZSM5 catalyst. The kinetic model used composed of a cycle methylation from C_4^- through C_5^- to C_6^- and further to C_7^- . The beta scission of C_6^- and C_7^- caused propylene production. Some experiments were carried out using monolithic and packed bed reactors for estimation of the kinetic parameters in the process. Mihail *et al.* [9] developed a complex model for MTO process on a modified synthetic mordenite catalyst. The model contained individual steps up to 53 reactions and about 37 chemical species including radicals and molecules. Yuan *et al.* [10] investigated methanol conversion reaction and coke deposition over SAPO-34 catalyst in a microscale fluidized bed reactor, which showed some interesting results in their temperature-programmed experiments. The experiments started with methanol, which was fed to the reactor at 250°C, but the hydrocarbon products generated in the temperature range of 250-300°C were negligible. The conversion of methanol increased from temperature of 300°C and reached a peak conversion at 325°C and then dropped when the temperature was 350°C. When the temperature further went beyond 350°C, the conversion of methanol increased continuously. Park *et al.* [11] formulated detailed kinetic models at the elementary step level for the methanol to olefin process over HZSM-5 catalyst with a Si/Al ratio of 200. Starting from plausible mechanisms, the formation of primary products was modelled rigorously by means of Hougen-Watson approach. The generation of higher olefins was expressed in terms of carbenium ion mechanisms. A computer algorithm was used to generate the reaction network. The rate coefficient of each elementary step was formulated according to single-event approach. The number of single events for each elementary step was calculated from the structure of the activated complex determined by quantum chemical calculations. Activation energies for each elementary step were obtained through the Evans-Polanyi relation that accounts for various energy levels of carbenium ions and olefin isomers. The single event kinetics combined with the Evans-Polanyi relation provided a tremendous reduction in the number of parameters estimated, which was later restricted by thermodynamic constraints.

It can be noticed from the literature review that research studies involving modelling and simulation using process simulators on the subject matter, which is methanol-to-olefin is very scarce. Therefore, this work has been carried out to contribute to this area by applying Aspen HYSYS to model and simulate a methanol-to-olefin process taking the production of butene as a case study. In addition, the economic viability of the process was analysed.

2. Methodology

The methanol-to-butene process of this work was accomplished using a model developed in Aspen HYSYS [12] environment as described below.

2.1. Process Model Development

The development of the process model was carried out with the aid of Aspen HYSYS process simulator through the following stages:

- 1. Component selection:** The chemical components involved in the process were added to the model from Aspen HYSYS database, and they were:
 - Methanol
 - Dimethylether
 - 1-Butene
 - Water
- 2. Thermodynamic Package:** Peng-Robinson Stryjek-Vera equation of state was chosen as the thermodynamic package.
- 3. Flowsheet Development:** The flowsheet of the process was developed in a step-by-step approach in the Aspen HYSYS flowsheeting environment thus:
 - Step 1: A *Feedin* stream was created from the palette of the simulator and added to a heater (E-100) that was picked from the palette as well, and a *Feedout* stream was also created and



added to the heater output. An energy stream (Qh1) was also added for the heater operation. The model developed in this step is shown in Figure 1.

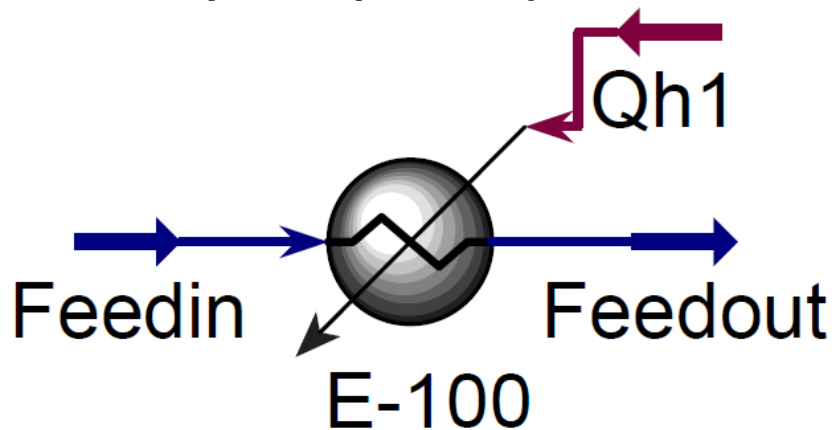


Figure 1: Aspen HYSYS model setup for step 1

- Step 2: The model was then modified by attaching the *Feedout* stream as the input of an equilibrium reactor while streams named *EquilreactorT* and *EquilreactorB* picked from the palette of Aspen HYSYS were the outputs (Figure 2). At this stage, the equilibrium reaction (Equation (1)) for the production of dimethyl ether from methanol was added to the reactor as well as the fluid package of the process simulation.

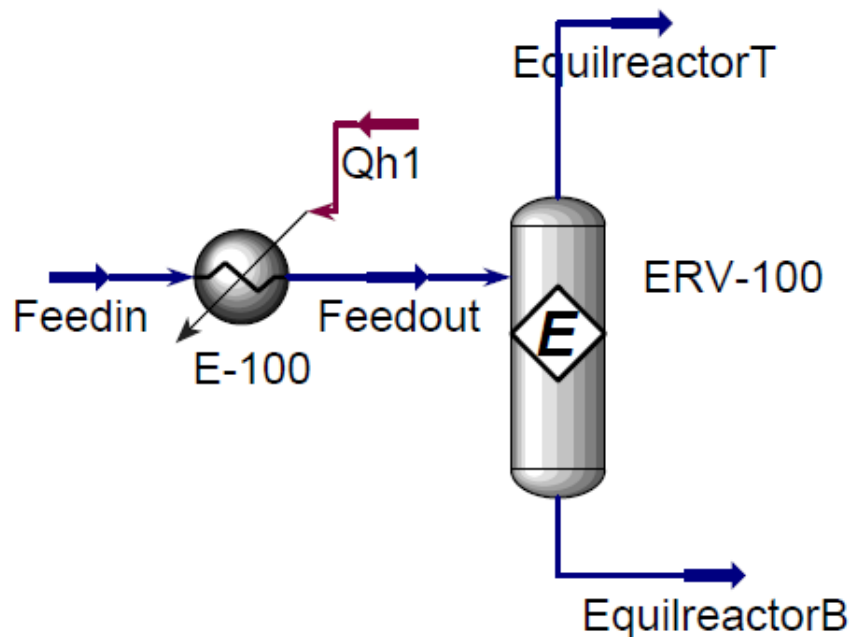
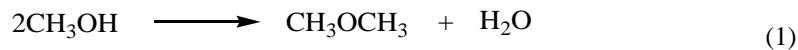


Figure 2: Aspen HYSYS model setup for steps 1-2

- Step 3: The model from stage 2 was further modified by passing the *EquilreactorT* stream of the equilibrium reactor to another heater (E-101), see Figure 3.



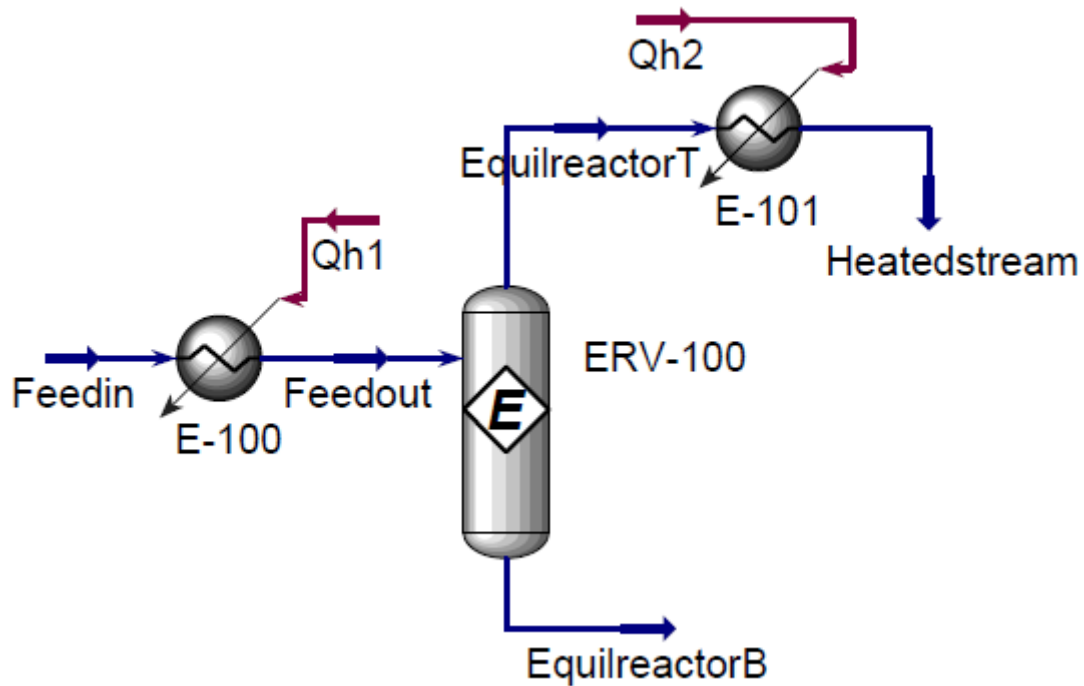


Figure 3: Aspen HYSYS model setup for steps 1-3

- Step 4: The heated stream of the heater (E-101) was fed into a plug flow reactor, which was also picked from the palette of the Aspen HYSYS, after which a stream named *PFRreactorout* was added to the output of the plug flow reactor as shown in Figure 4. The reaction given in Equation (2) was then attached to the reactor for butene production.

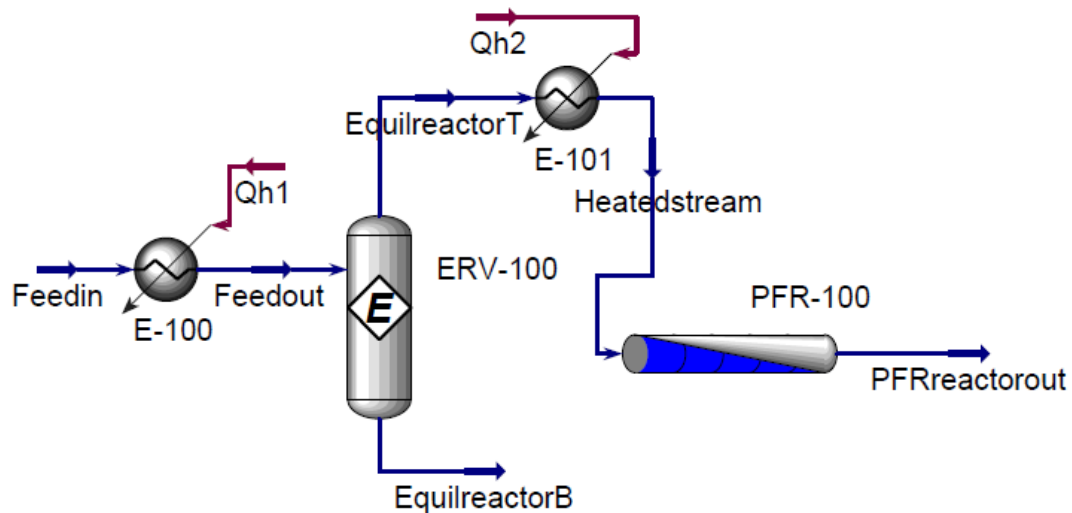
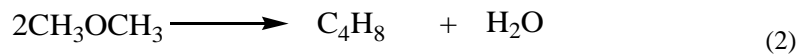


Figure 4: Aspen HYSYS model setup for steps 1-4

- Step 5: A cooler (E-101) was added to the flowsheet from Aspen HYSYS palette, and its input stream was made to be the *PFRreactorout* that was the output of the plug flow reactor. The exit stream of the cooler was tagged *Cooledstream* as shown in Figure 5.



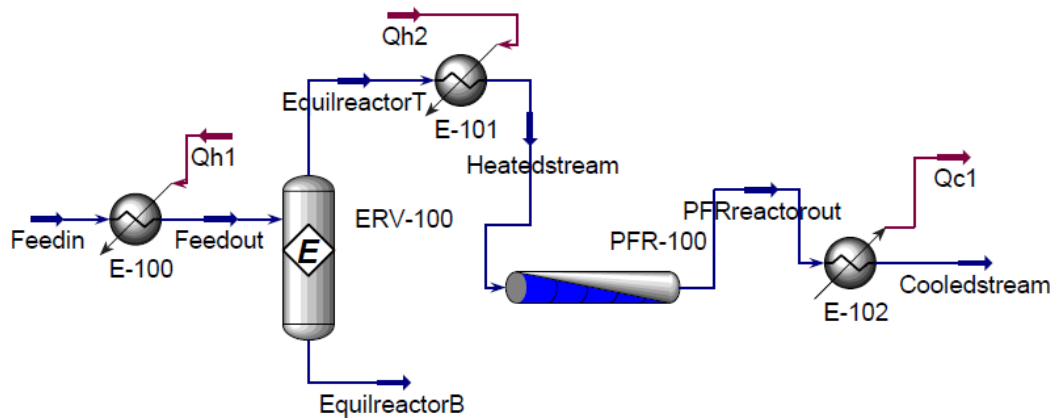


Figure 5: Aspen HYSYS model setup for steps 1-5

- Step 6: A separator (V-100) was added to the flowsheet from the palette and the *Cooledstream* was attached to the separator as its input, after which a top product stream (*Topstream*) and a bottom product (*Bottomstream*) were also added as the output streams, see Figure 6.

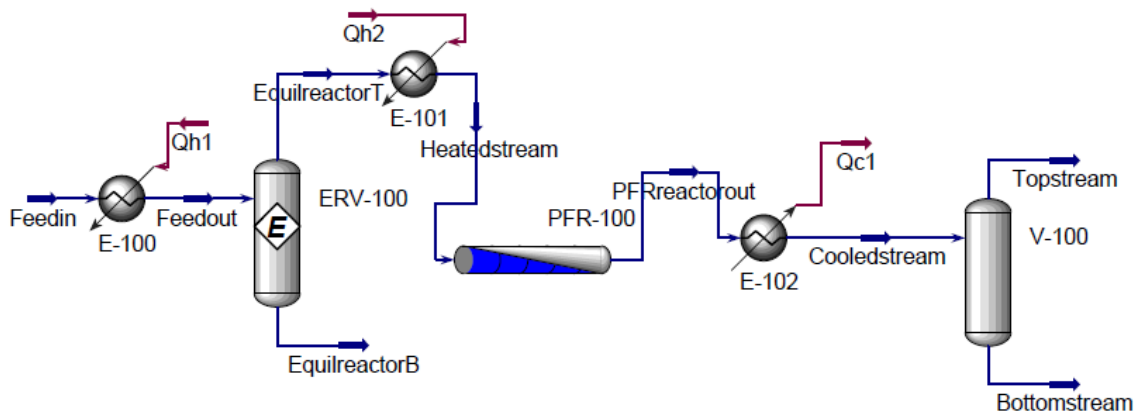


Figure 6: Aspen HYSYS model setup for steps 1-6

- Step 7: As seen in Figure 7, a cooler (E-102) was added from the palette to the flowsheet and the *Topstream* of the separator was inputted into it. Another stream called *Cooledproduct* was added to the flowsheet as well, to display the output stream of the cooler.

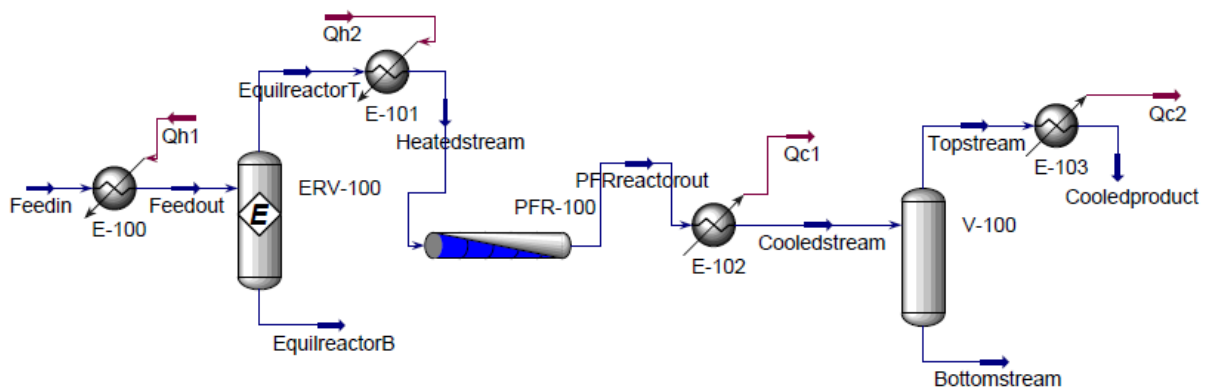


Figure 7: Aspen HYSYS model setup for steps 1-7



- Step 8: A tank (V-101) was added to the model setup for collecting the cooled liquid product. The input of the tank was the *Cooledproduct* while its vapour and liquid outputs were named *Tankvapour* and *Tankliquid* respectively. This was taken to be the final stage of the model setup (Figure 8) for butene production from methanol.

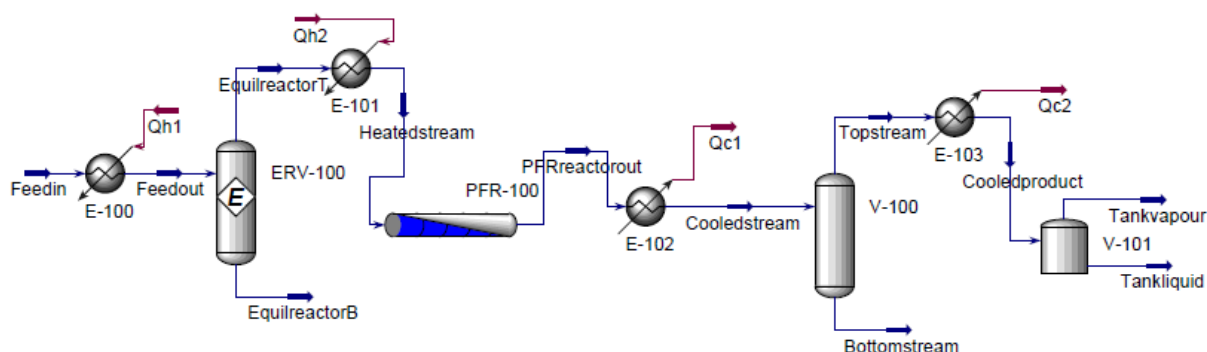


Figure 8: Aspen HYSYS model setup for the production of butene from methanol

4. **Feed Stream Specification:** The conditions for the feed stream, given in Table 1, were entered into the feed stream appropriately.

Table 1: Feed stream specification

Parameter	Value
Temperature (°C)	25
Pressure (atm)	1
Total Flow (mL/min)	35
Methanol mole fraction	1

5. **Equipment Specification:** The dimensions of the plug flow reactor were specified as given in Table 2.

Table 2: Plug flow reactor dimensions

Plug flow reactor dimension	Specification
Total Volume (m ³)	3.5
Length (m)	3.0

6. **Reaction Specification:** The kinetic data, where were activation energy and frequency factor, used for plug flow reaction given in Equation (2) were obtained from the literature [13], and they are shown in Table 3.

Table 3: Reaction kinetics data [13]

Reaction kinetic parameter	Value
Activation Energy (J/mol)	63590
Frequency Factor	4.70×10^5

3. Results and Discussion

The steady-state results obtained from the simulation of the developed model for the methanol-to-butene production process are given in Tables 4 - 6.

Table 4 shows the molar composition of the product. As can be seen from the table, the desired product of all the components, which was butene, was discovered to have the highest mole fraction in the final product of the process. This was an indication that the production of butene from methanol was accomplished in the process successfully.



Table 4: The composition of the final product

Component	Mole fraction
Methanol	0.0001
Dimethyl ether	0.0000
Butene	0.8424
Water	0.1574

The conditions of the final product of the methanol-to-butene process are given in Table 5. It can be deduced from the table that the product was liquid in nature because its vapour phase fraction was found to zero. Also noticed from the results was that the product could be obtained at normal atmosphere as the pressure of the product stream was 1 atm.

Table 5: The conditions of the final product

Parameter	Value
Vapour / Phase Fraction	0.00
Temperature [$^{\circ}\text{C}$]	-6.42
Pressure [atm]	1.00
Molar Flow [gmole/min]	0.22
Mass Flow [g/min]	10.84
Std Ideal Liq Vol Flow [mL/min]	17.84
Molar Enthalpy [kJ/kgmole]	-66654.33
Molar Entropy [kJ/kgmole- $^{\circ}\text{C}$]	10.89
Heat Flow [kJ/s]	-0.24
Liq Vol Flow @Std Cond [mL/min]	17.42

The properties of the final product stream and those of its liquid phase are shown in Table 6, and it could be noticed from the table that the liquid phase material obtained from the product was actually butene because some of the properties given in the table were observed to have very close values to those of butene, as obtained in the literature [12]. For instance, the molecular weight of butene is 56.11 kg/kgmole while the one obtained as the property of the liquid phase in the final product was 56.10. The standard ideal liquid mass density is another property confirming the authenticity of the butene obtained as the liquid product of this process.

Table 6: The properties of the final product stream

Property	Final Product	Liquid Phase
Molecular Weight[kg/kgmole]	50.11	56.10
Molar Density [kgmole/m ³]	12.72	11.11
Mass Density [kg/m ³]	637.36	623.09
Actual Volume Flow [mL/min]	17.01	16.42
Mass Enthalpy [kJ/kg]	-1330.24	-450.84
Mass Entropy [kJ/kg- $^{\circ}\text{C}$]	0.22	0.07
Heat Capacity [kJ/kgmole- $^{\circ}\text{C}$]	114.47	122.11
Mass Heat Capacity [kJ/kg- $^{\circ}\text{C}$]	2.28	2.18
LHV Molar Basis (Std) [kJ/kgmole]	2142973.93	2543522.31
HHV Molar Basis (Std) [kJ/kgmole]	2287631.98	2707551.91
HHV Mass Basis (Std) [kJ/kg]	45655.08	48259.09
LHV Mass Basis (Std) [kJ/kg]	42768.09	45335.45
Phase Fraction [Mass Basis]	0.00	0.94
Phase Fraction [Actual Volume Basis]	0.00	0.96
Cost Based on Flow [Cost/s]	0.00	0.00
Average Liquid Density [kgmole/m ³]	12.13	10.58
Specific Heat [kJ/kgmole- $^{\circ}\text{C}$]	114.47	122.11
Std. Gas Flow [STD_m ³ /h]	0.31	0.26
Std. Ideal Liq. Mass Density [kg/m ³]	607.74	593.80
Act. Liq. Flow [mL/min]	17.01	16.42



Watson K	13.16	13.16
C _p /(C _p - R)	1.08	1.07
C _p /C _v	1.41	1.46
Kinematic Viscosity [cSt]	0.33	0.30
Liquid Mass Density (Std. Cond) [kg/m ³]	622.48	598.17
Liquid Volume Flow (Std. Cond) [mL/min]	17.42	17.10
Liquid Fraction	1.00	1.00
Molar Volume [m ³ /kgmole]	0.08	0.09
Phase Fraction [Molar Basis]	0.00	0.84
Thermal Conductivity [W/m-K]	0.11	0.10
Viscosity [cP]	0.21	0.18
C _v (Semi-Ideal) [kJ/kgmole-°C]	106.16	113.80
Mass C _v (Semi-Ideal) [kJ/kg-°C]	2.12	2.03
C _v [kJ/kgmole-°C]	81.23	83.56
Mass C _v [kJ/kg-°C]	1.62	1.49
Reid VP at 37.8 °C [atm]	4.30	4.30
True VP at 37.8 °C [atm]	4.37	4.31
Liquid Volume Flow – Sum (Std. Cond) [mL/min]	17.71	17.10

Having confirmed that the production of butene from methanol could be accomplished successfully in the process that was simulated, the specifications of the pieces of equipment involved were then carried out, and the results obtained for the specifications are given in Tables 7 – 11.

Table 7 shows the results of the specification of the heat exchangers of the process. Based on the information obtained from the results, even though the heat exchangers had the same tube outside diameter, tube pitch and tube length extended, their available areas for heat transfer were not the same with one another. This was observed to be due to the different nature and the conditions of the components involved in the heat transfer operations.

Table 7: Specification of the heat exchangers

Parameter	Heater 1	Heater 2	Cooler 1	Cooler 2
User tag number	E-100	E-101	E-102	E-103
Heat transfer area [m ²]	0.00110	0.00742	0.00308	0.00503
Tube design gauge pressure [kPag]	760.55	3001.42	415.80	243.42
Tube design temperature [°C]	192.11	257.00	700.32	121.11
Tube operating temperature [°C]	164.33	229.22	35.00	-29.80
Tube outside diameter [m]	0.03	0.03	0.03	0.03
Shell design gauge pressure [kPag]	473.25	1967.17	243.42	128.50
Shell design temperature [°C]	121.11	227.78	700.32	121.11
Shell operating temperature [°C]	60.00	200.00	672.54	55.00
Tube length extended [m]	6.10	6.10	6.10	6.10
Tube pitch [m]	0.03	0.03	0.03	0.03
Number of tube passes	1	1	1	1
Number of shell passes	1	1	1	1

The specifications of the equilibrium reactor that was used to produce the intermediate product (dimethyl ether) are shown in Table 8. The dimensions obtained for the reactor were found to be moderate and appropriate for the production carried out in the process of this work. Besides, it was clear from the specifications that only half of the total volume of the reactor was filled with process liquid. This was found to be very favourable to the process as to avoid overflow, in case there is any turbulence, during the reaction process.



Table 8: Specification of the equilibrium reactor

Parameter	Value
Vessel Diameter [m]	0.57
Height [m]	0.85
Liquid Volume Percent [%]	50.00

Table 9: Specification of the plug flow reactor

Parameter	Value
User tag number	PFR-100
Vessel diameter [m]	1.22
Vessel tangent to tangent height [m]	3.05
Design gauge pressure [kPag]	103.43
Total packing height [m]	2.74

Table 10: Specification of the separator

Parameter	Value
User tag number	V-100
Vessel diameter [m]	0.91
Vessel tangent to tangent height [m]	3.66
Design gauge pressure [kPag]	103.43

Table 11: Specification of the storage tank

Parameter	Value
User tag number	V-101
Vessel diameter [m]	0.46
Vessel height [m]	0.30
Design gauge pressure [kPag]	103.43

Shown in Table 9 are the specifications of the plug flow reactor, which was used to carry out the conversion of dimethyl ether to butene, of the process. According to the results obtained in this case, the plug flow reactor was found to be suitable for the reaction carried out inside it because the dimensions were found appropriate and suitable.

Table 12: Summary of economic analysis of the plant

Description	Value
Total Capital Cost [USD]	2,832,250
Total Operating Cost [USD/Year]	970,119
Total Utilities Cost [USD/Year]	35,629.1
Desired Rate of Return [Percent/Year]	20
Equipment Cost [USD]	118,700
Total Installed Cost [USD]	424,700

Furthermore, the results given when the specifications of the separator and the storage tank of the process were simulated were as shown in Tables 10 and 11, respectively. The results shown in the tables also indicated the suitability of the developed model for methanol-to-butene process because their dimensions too were found to be good and appropriate for this kind of process setup.

The summary of the results obtained from the economic analysis of the developed prototype plant of the methanol-to-butene process carried out with the aid of Aspen HYSYS were as given in Table 12. The results contained in the table pointed to the fact that the process would be economically viable because the value obtained for the rate of return indicated that any amount spent in setting up the plant could be recovered within five years.



4. Conclusion

The results obtained from the simulation of the methanol-to-butene process revealed that butene could be produced successfully because the developed model was able to converge when simulated to give a mole fraction of butene coming out of the plug flow reactor to be 0.3329 and that obtained after the separation operation had been carried out to be 0.8424. The specifications of the pieces of equipment used to obtain the high mole fraction (0.8424) of the butene from methanol showed that the plant could be easily set up because the dimensions were moderate enough for a process of this nature. Furthermore, the economic viability of the process was seen from the rate of return of the process that was estimated to be 20%, which was found to be an indication that five years would be enough for the amount invested on the plant to be recovered. It is recommended that an experiment on a pilot scale should be carried out to practically validate the steady state results obtained in this work. Also, the process should be integrated by combining the equilibrium reactor, the plug flow reactor and the separator as a single vessel like that of a reactive distillation column that has been described by different researchers [14-38] to be more economical than this conventional approach.

Acknowledgement

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

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