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Sensitivity Analysis of a Methanol-to-Propene Process Using Aspen HYSYS

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Abstract: *In this work, the sensitivity analysis of a process for the production of propene from methanol, otherwise known as methanol-to-propene (MTP) process, has been carried out. The study was accomplished by developing a model of the process involving an equilibrium reactor, a kinetic reactor, two pieces of cooling equipment and a separator with the aid of Aspen HYSYS using Wilson model as the fluid package. The selected input variables were feed flow rate, temperature and pressure that were varied and the output variables, which were the mole fractions of the process components, were recorded during the simulation. The results obtained from the sensitivity analysis involving variations in the feed flow rate revealed the validity of the developed process model because the output variables were found not to change with changes in the feed flow rate under the same temperature and pressure. Furthermore, the results showed the sensitivity of the process towards feed temperature at all the exits (reactor 1, reactor 2 and final outputs) and feed pressure at the final output considered for the process.*

Keywords*: Methanol-to-propene, dimethyl ether (DME), sensitivity analysis, Aspen HYSYS*

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NOMENCLATURE

Cooler1	Cooling equipment 1
Cooler2	Cooling equipment 2
Cooler2Out	Output of cooler 2
Qc1	Heat duty of cooler 1
Qc2	Heat duty of cooler 2
Reactor1	Equilibrium reactor
Reactor1Bottom	Bottom product of reactor 1
Reactor1Top	Top product of reactor 1
Reactor2	Plug flow reactor
Reactor2Out	Output of reactor 2
SeparatorBottom	Bottom product of separator
SeparatorTop	Top product of separator

I. Introduction

The global economy in recent decades has become more interconnected and dependent; thereby, providing new sources of industrial valuable products and energy has become deeply critical to remain competitive in meeting market demands. With the current energy demand far surpassing energy supply, this focus seems more relevant than ever. In recent years, methanol-to-olefins (MTO) process has received wide attention as it provides an indirect route in reaching that goal [1].

The global energy scene is largely based on fossil fuel resources, which are oil, coal and natural gas. They represent nearly 80% of the global energy consumption with petroleum being the highest (35%) [2].Although they may still seem abundant, especially in the producing regions, these fossil fuel reserves will in a more or less close future disappear: 40 years expected for oil, 70 years for natural gas and around 170 years for coal at the present rate of consumption [3].

Oil serves as a very important raw feedstock for the production of numerous key petrochemical building blocks. With the continuous increase in the rise in energy demand, various technologies producing liquid hydrocarbon fuels play important roles in the global energy chain and, hence, are very attractive. Biomass, natural gas, carbon dioxide and coal appear to be alternative carbon sources, from this perspective [2].

Because of the oil crisis in the early 1970s, the methanol-to-hydrocarbons (MTH) technology became a strong tool to produce either gasoline, as in methanol-to-gasoline - MTG process, or olefins, as in methanol-to-olefins - MTO process [2].

In 1973, the development of ZSM-5 zeolite alongside its unique catalytic properties by researchers at the Mobil Oil company enabled them to discover, by accident, the MTG process, which was ready to be commercialized in 1985 [4].

The MTO process has been widely promoted and studied with respect to the MTG process during the last decade. This is due to the strong demand of lower olefins, especially regarding ethylene and propylene because the world propylene consumption is forecasted to increase by close to 5% per year in coming years, and that of ethylene is expected to experience growth rate of about 4% per year [3].This driving force pushed scientists to the development of methanol-to-propene (MTP) technology [2].

Propene, otherwise referred to as propylene, is an important building blocks widely used as a feedstock and as a precursor for a variety of polymers and chemical intermediates, like polypropylene, cumene, propylene oxide, acrolein, acrylonitrile, isopropyl alcohol and other miscellaneous intermediates. These compounds are applied in a large range of industries which includes automotive, packaging and electronic industries [2].

Traditional industrial production of propene is performed by methods such as steam cracking, fluidized catalytic cracking (FCC) and propane dehydrogenation. Besides the availability of low-cost methanol, such expected growth in propene demand makes the MTP process viable. Currently, the Lurgi MTP process owned by the Lurgi Company, involving the ZSM-5 catalyst, developed by Süd-Chemie has been commercialized [2].

The MTP process allows a high selectivity in propene (about 70%) at complete methanol conversion with gasoline range compounds as by-products and slow deactivation rate. This high selectivity in propylene is related to an efficient combination of a very selective and stable catalyst and a most suitable reactor configuration. Thus, a high selectivity is normally achieved. Another important parameter in the commercial set-up is the recycling of olefins, which enables the maximization of propene selectivity [2].

Besides being a raw material for propene production, methanol is a popularly used feedstock in the chemical industries. It can be made using a variety of different chemical feedstock (petroleum, syngas, and coal) and used to produce a range of value-added chemicals and fuels including other olefins, gasoline, dimethyl ether, methyl *tert* butyl ether, acetic acid, and formaldehyde [2].

The literature review carried out revealed that researches concerning the study of the parameters affecting this process through modelling and simulation is very scarce, and this is affecting further and more rigorous theoretical study of the process. This work has been carried out to bridge this gap by applying Aspen HYSYS process simulator to carry out sensitivity analysis on the process by investigating the behaviour of a methanol to propene process in response to some input variables.

II. Methodology

This research work was carried out by developing a model for the methanol-to-propene process with the aid of Aspen HYSYS [5] using the steps outlined thus.

2.1 Definition of Methanol to Propylene Mechanism

The initial step of the methanol-to-propene process is the dehydration of methanol to dimethyl ether (DME) as shown in Equation (1), which reacted further to form propene, as given in Equation (2). In the real sense, small amounts of other olefins, alkanes and some aromatics are also produced by the process.

$$2CH_3OH \leftrightarrow CH_3OCH_3 + H_2O \quad (1)$$

$$3CH_3OCH_3 \rightarrow 2C_3H_6 + 3H_2O \quad (2)$$

2.2 Components and Fluid Package Selection

The chemical components involved in the process were chosen from the databank of Aspen HYSYS components list, which were methanol - CH_3OH, dimethyl ether (DME) – CH_3OCH_3, water - H_2O, and propene – C_3H_6, and they were associated with Wilson model as the fluid package for the estimations of transport and physicochemical properties.

2.3 Flowsheet Development

To develop the flowsheet of the methanol-to-propene process, the pieces of equipment (one equilibrium reactor, one plug flow reactor, two coolers and one separator) involved as well as the feed and product streams were chosen from the object palette of the process simulator and placed on the Aspen HYSYS simulation environment. Thereafter, they were joined together with the intermediate streams to form the model of the process shown in Figure 1.

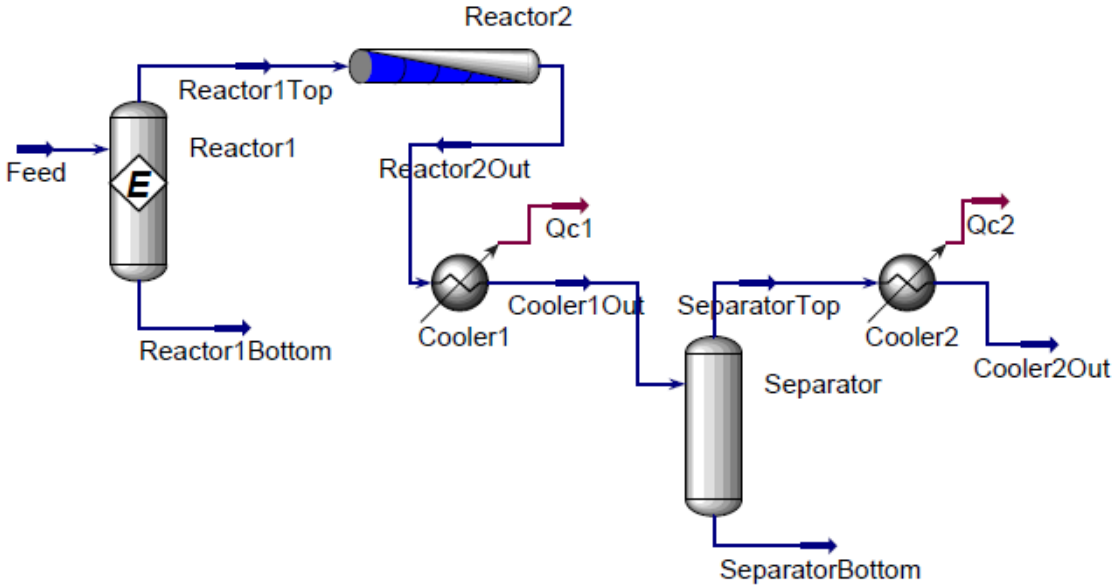

Figure 1: Aspen HYSYS flowsheet of the methanol-to-propene process

2.4 Feed Stream Specification

After developing the flowsheet of the process, the parameters of the feed stream (Table 1) were entered before simulating it for steady-state convergence.

Table 1: Methanol-to-propene steady-state feed stream conditions

Stream Name	**Feed**
Temperature (^oC)	25
Pressure (atm)	1
Total Flow (mL/min)	45
Methanol purity (mol%)	1

2.5 Sensitivity Analysis

Sensitivity analysis, which is the study of how uncertainty in the output of a model can be attributed to different sources of uncertainty in the model input, was carried out in this research work to investigate how different values of some independent variables affected some dependent variables under a given set of conditions. This technique was used, in this work, with specific variables and within specific boundaries outlined below:

Independent variables:
Flow rate
Pressure
Temperature

Dependent variables:
Methanol master comp mole fraction
Dimethyl ether master comp mole fraction
Water master comp mole fraction
Propene master comp mole fraction

Low bound:
For flow rate: 45 mL/min
For temperature= 25^oC
For pressure = 1 atm

High bound:
For flow rate: 100 mL/min

For temperature= 135 ^{o}C
For pressure = 2atm

Step size:
For flow rate: 2.5 mL/min
For temperature= 5 ^{o}C
For pressure = 0.05atm

The sensitivity analysis of the methanol-to-propene process was accomplished by opening the case study from the simulation window in the flow sheeting environment, adding new case studies and inputting the data of the variables given above appropriately and accordingly.

III. Results and Discussion

The output obtained from the steady-state simulation of the Aspen HYSYS model developed for the methanol-to-propene process indicated that it (the system) could converge with mole fractions of the components present in the final product being 0.0025, 0.0003, 0.1009and 0.8963for methanol, dimethyl ether, water and propene, respectively.

Furthermore, the results obtained from the sensitivity analysis simulation are given in Figures 2 – 10. Figure 2 shows the responses of the mole fraction of the process components (methanol, dimethyl ether, water and propene) obtained as the output of the reactor 1 when the flow rate was varied while keeping the feed temperature and pressure constant. From the figure, it was noticed that the mole fractions of the components were constant throughout the flow rate interval used for the simulation with dimethyl ether having the highest value, in this case, because it was the main product of the reaction occurring in the reactor 1.

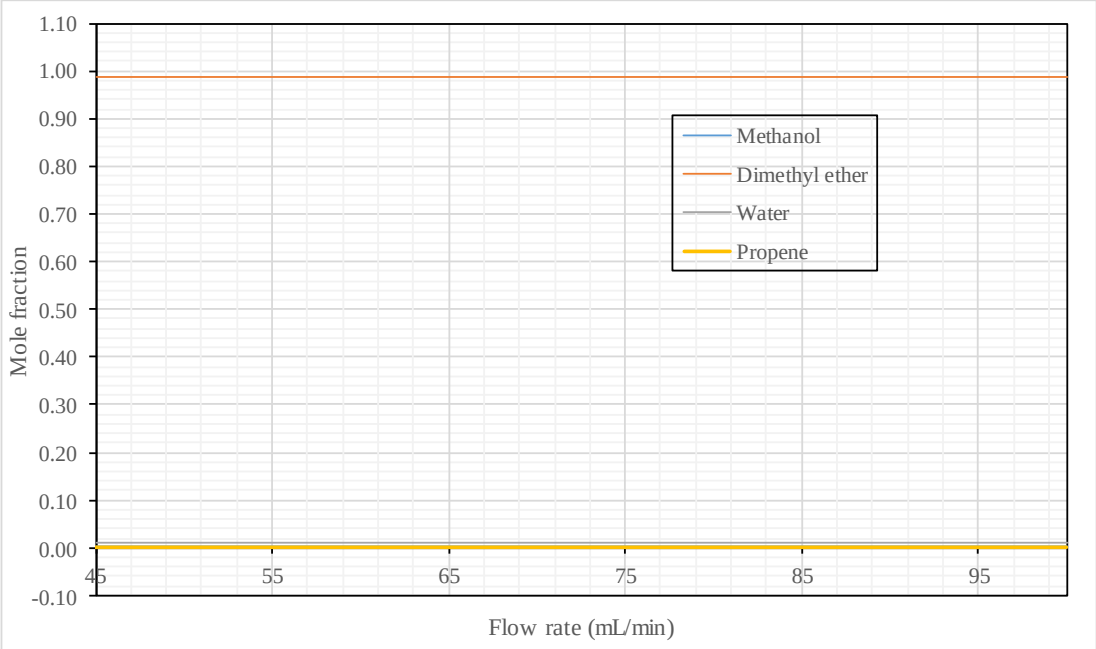

Figure 2. Component mole fraction responses to changes in feed flow rate for reactor 1 top product (T = 25 ^{o}C, P = 1 atm)

Shown in Figure 3 are the mole fraction responses involved in the output of reactor 2, which was used to produce the desired product (propene). The observation made in this case revealed that the mole fractions of the components are also constant within the flow rate range considered. However, in this case, water had the highest mole fraction followed by propene. The mole fraction of dimethyl ether and methanol were found to be negligible in the output of this reactor because methanol was already consumed in reactor 1 to produce dimethyl ether as the main product there (in reactor 1) and that of dimethyl ether too has been consumed in reactor 2 to give propene as the desired product of the process.

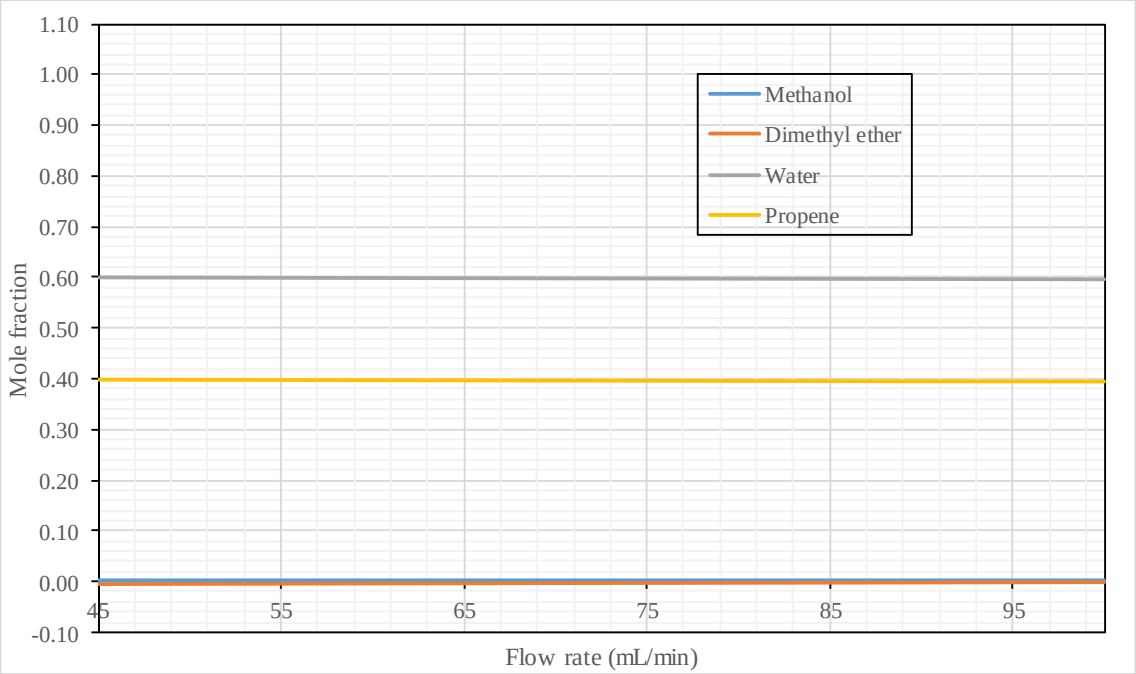

Figure 3. Component mole fraction responses to changes in feed flow rate for reactor 2 product (T = 25 ^{o}C, P = 1 atm)

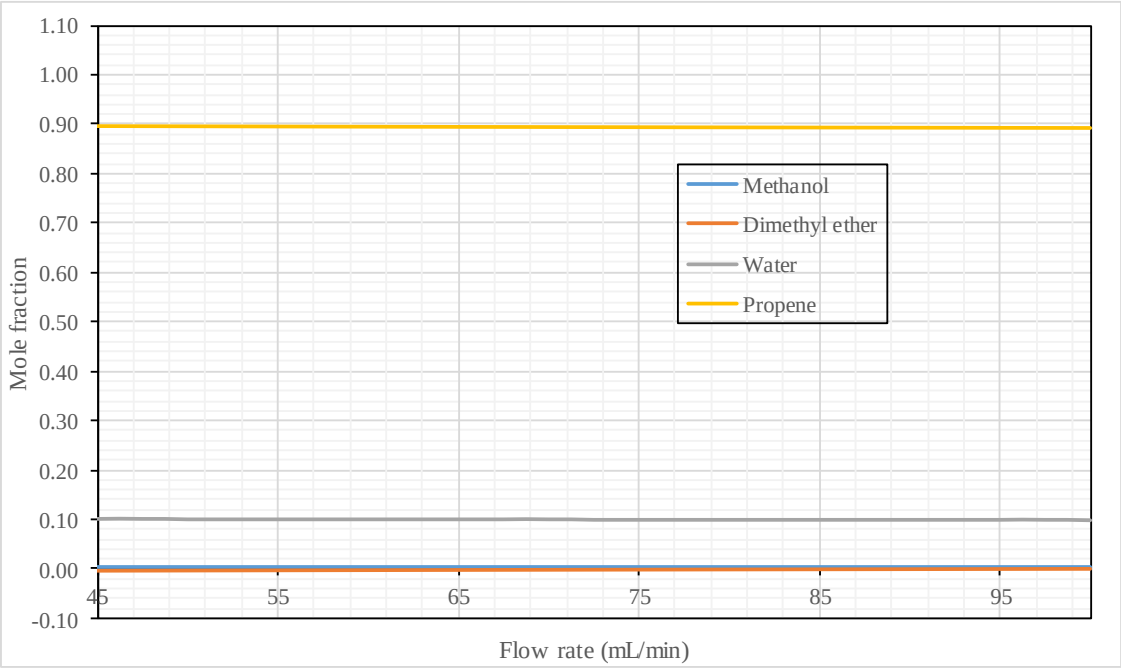

Figure 4. Component mole fraction responses to changes in feed flow rate for final product (T = 25 ^{o}C, P = 1 atm)

The mole fraction responses of the components to changes in the feed flow rate, as obtained from the final product stream of the process, are given in Figure 4. It was observed from the results shown in the figure that propene had the highest mole fraction in the final product because separation had been carried out, although the responses were still found to be constant throughout the range of the feed flow rate considered.

The results given in Figures 2 – 4 were obtained to show the validity of the developed Aspen HYSYS model of the methanol-to-propene process, and this has been shown since the mole fraction responses were constant through the range of the feed flow rate used at different points of the process. This also pointed to the fact that the process would be easily scaled up as the variation in the feed flow rate did not affect the nature of the response given by each of the components at each point of the process flowsheet.

Given in Figure 5 are the component mole fraction responses obtained from the exit of reactor 1 of the methanol-to-propene process to changes in feed temperature. It can be seen clearly from the results shown in the figure that the components responded to the changes in the temperature. Also, it was discovered that, for the feed temperature of 25 to about 65 ^{o}C, dimethyl ether had the highest mole fraction in the output of reactor 1. Its mole fraction was found to be equal to that of water for the temperature range of about 70 – 135 ^{o}C in the range that was considered. The mole fraction response of the process feed (methanol) was the lowest in the output of reactor 1; this was an indication that there was good conversion occurring in the reactor. Of course, the desired product, propene, was not yet produced in the process at this point, and that was why its mole fraction was found to be zero throughout on the figure.

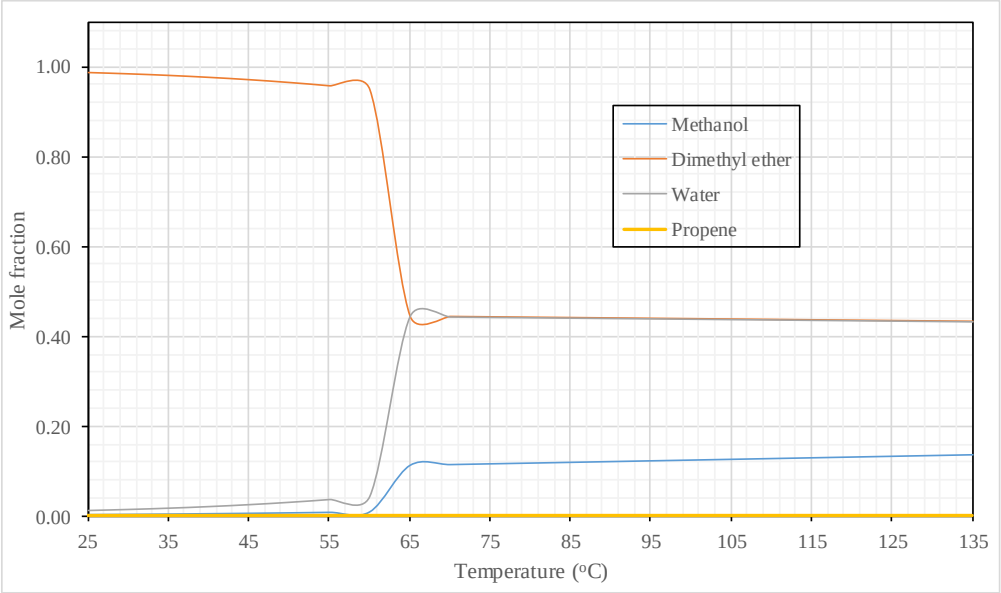

Figure 5. Component mole fraction responses to changes in feed temperature for reactor 1 top product (F = 45 mL/min, P = 1 atm)

Figure 6 shows the responses of the components in the output of reactor 2 with variation in feed temperature. According to the results shown in the figure, the components were able to respond to the changes that occurred in the feed temperature with water having the highest mole fraction followed by propene, throughout the range used. The mole fraction of dimethyl ether was approximately zero in the output of reactor 2 because it had been consumed in this reactor for the production of propene.

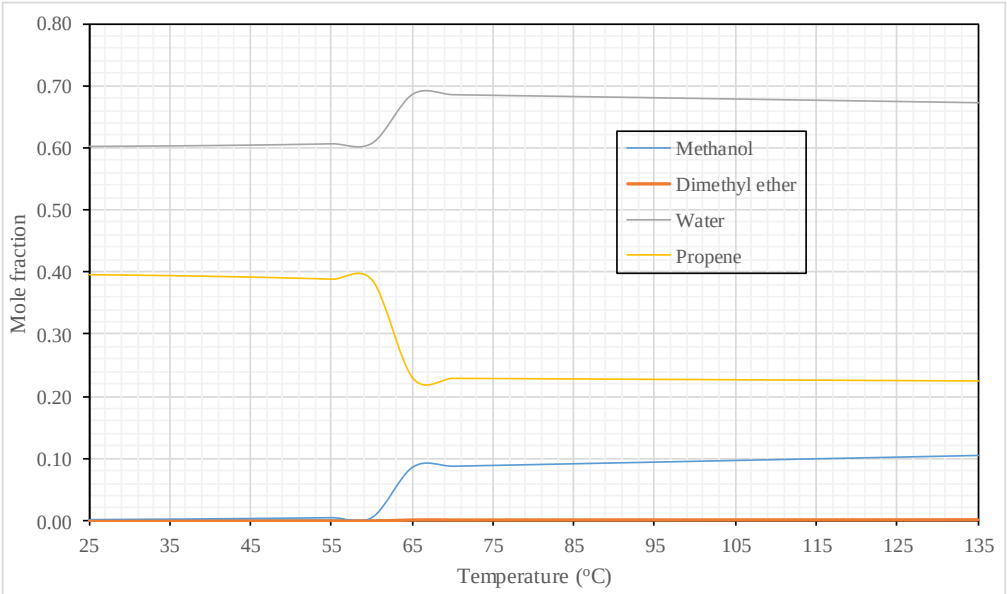

Figure 6. Component mole fraction responses to changes in feed temperature for reactor 2 product (F = 45 mL/min, P = 1 atm)

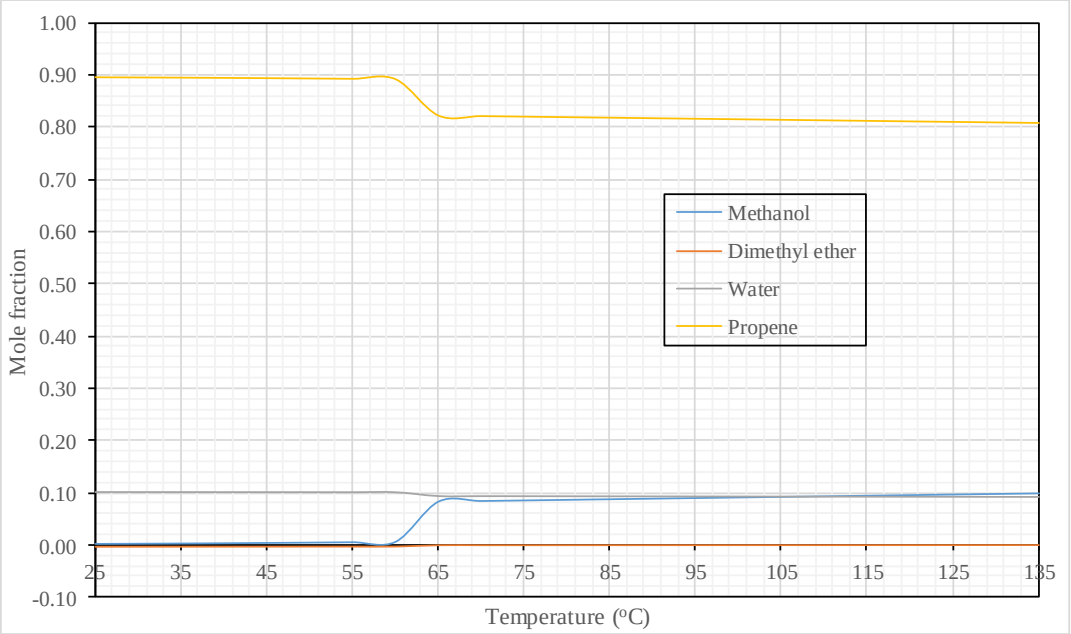

Figure 7. Component mole fraction responses to changes in feed temperature for final product F = 45 mL/min, P = 1 atm)

The responses obtained as the mole fractions of the components after separation had been carried out in order to obtain high purity of the desired product (propene) were as given in Figure 7. The responses given in this case showed that propene had the highest mole fraction in the final product of the process while the mole fractions of the other components were very small. This is pointing to the success of the separation carried out.

The mole fraction responses of the components to changes in feed pressure are given in Figure 8 for the output of reactor 1 of the process. It was discovered from the figure that the components in the output of reactor 1 were not responding to changes in the feed pressure. In other words, the feed pressure was not having any effect on the components present in the output of reactor 1. However, dimethyl ether was discovered to have the highest mole fraction throughout the change that occurred in the feed pressure. The mole fractions of the other components were approximately negligible at that output. Propene was not present at all in the output of the reactor 1.

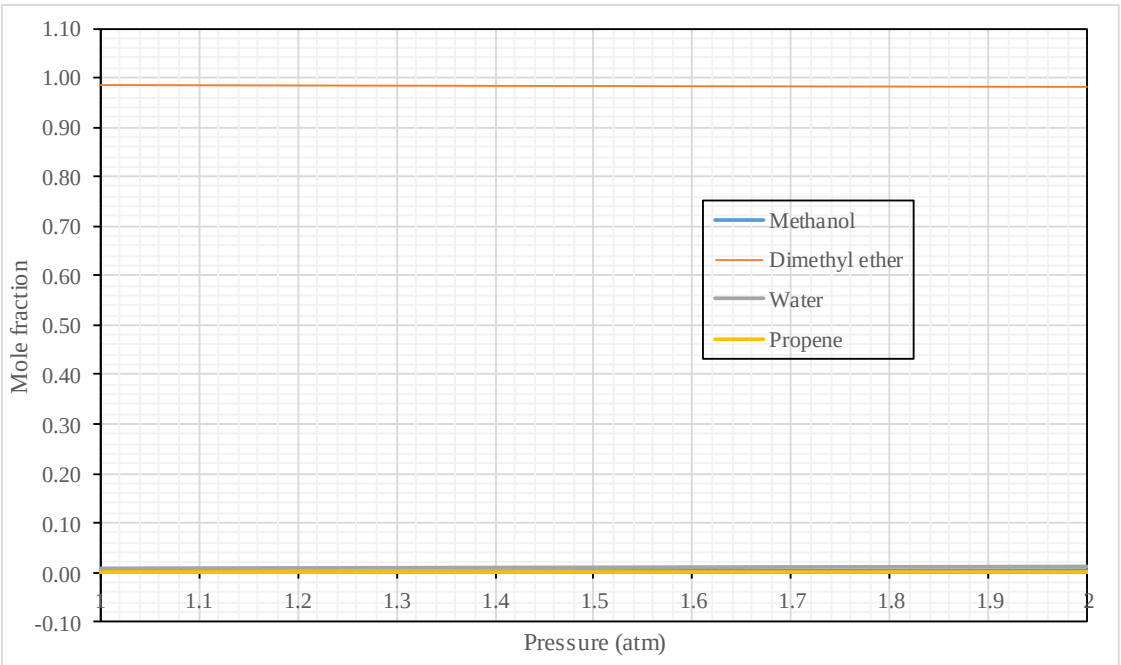

Figure 8. Component mole fraction responses to changes in feed pressure for reactor 1 top product (T = 25 °C, F = 45 mL/min)

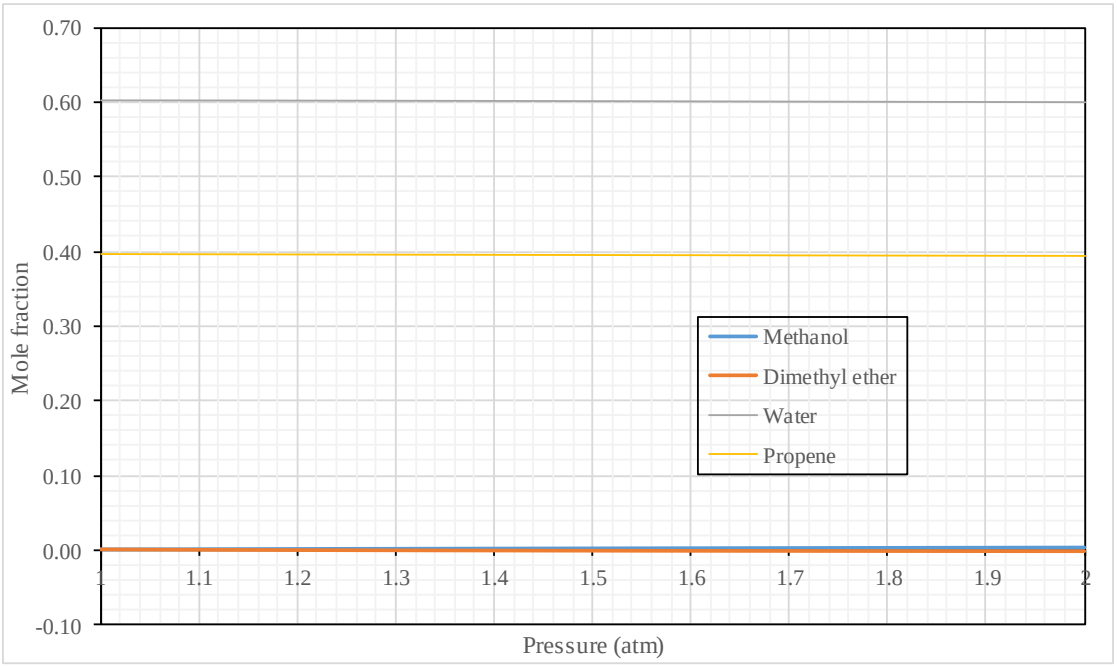

Figure 9. Component mole fraction responses to changes in feed pressure for reactor 2 product (T = 25 ^{o}C, F = 45 mL/min)

Figure 9 gives the responses of the component mole fractions for the output of reactor 2 with varying feed pressure. The responses obtained in this result were also found to be constant throughout the range of the feed pressure considered, though, water was found to possess the highest mole fraction, in this case, followed by propene.

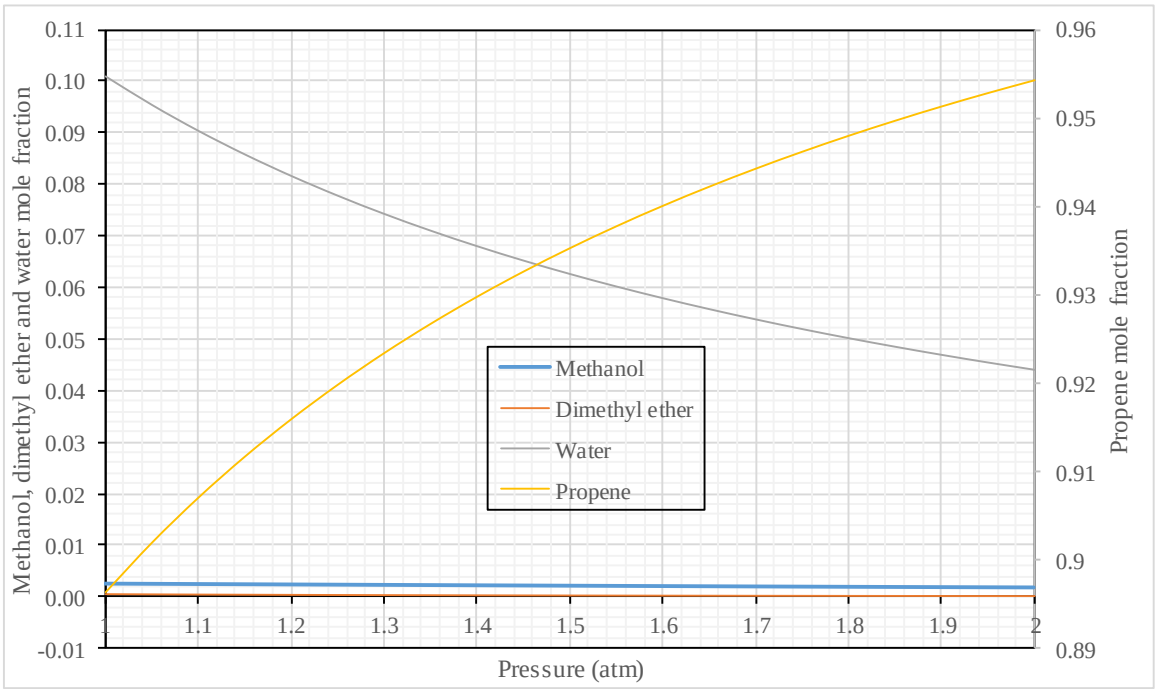

Figure 10. Component mole fraction responses to changes in feed pressure for final product (T = 25 ^{o}C, F = 45 mL/min)

The responses of the component mole fractions to changes in feed pressure for the final product of the process are shown in Figure 10. In this case, the mole fraction responses of the product components of the process, which were propene and water, were found not to be constant, in contrast to how they were obtained for the outputs of reactors 1 and 2. It was also noticed from the results given in Figure 10 that the mole fraction response of propene increased while that of water was observed to decrease with increase in feed pressure. The

mole fraction responses of both methanol and dimethyl ether were found to be constant and almost negligible throughout the feed pressure range considered in this work.

IV. Conclusion

The results obtained from the sensitivity analysis carried out with the aid of Aspen HYSYS on methanol-to-propene process using the feed flow rate as the input variable and the mole fractions of the components as the output variables revealed that the developed model was a valid one because the changes in the feed flow rate under the same temperature and pressure did not result in significant changes in the output variables at different points of the process outputs. Furthermore, it was discovered from the results that the process was sensitive to feed temperature at all the exits (reactor 1, reactor 2 and final outputs) considered. The responses of the process, especially those of propene and water, were seen to be significantly sensitive to feed pressure at the final product only. It is recommended that the process should be simulated using an integrated process known as reactive distillation because it allows the occurrence of reaction and separation in a single piece of equipment [6-26].

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References

[1]. Jean, L. (2005). Effect of Process Parameters on Methanol to Olefins Reactions over SAPO Catalysts. Master of Science Thesis. Auburn University, Auburn, Alabama, 116 pages.
[2]. Olomolehin, O.C. (2018). Modelling, Simulation and Sensitivity Analysis of a Methanol to Propylene Process Using Aspen HYSYS. Afe Babalola University, Ado-Ekiti, Ekiti State, Nigeria, 62 pages.
[3]. Olah, G.A., Goeppert, A. and Prakash, G.K.S. (2006). Beyond Oil and Gas: The Methanol Economy, 307 pages.
[4]. Stöcker, M. (2010). Methanol to Olefins (MTO) and Methanol to Gasoline (MTG), Chapter 22, Zeolites and Catalysis: Synthesis, Reactions and Applications. Wiley-VCH Verlag GmbH & Co. KGaA.
[5]. Aspen. (2015). Aspen HYSYS V8.8 [34.0.0.8909], Aspen Technology, USA.
[6]. Giwa, A, Giwa, SO, and Hapoglu, H. (2013). Adaptive neuro-fuzzy inference systems (ANFIS) modeling of reactive distillation process. ARPN Journal of Engineering and Applied Sciences, 8(7), 473-479.
[7]. Giwa, A. and Giwa, S.O. (2016). Modelling and simulation of a reactive distillation process for fuel additive production. Journal of Environmental Science, Computer Science and Engineering & Technology, Section C: Engineering & Technology. 5(1), 63-74.
[8]. Giwa, A. (2016). PI and PID control of a fuel additive reactive distillation process. ARPN Journal of Engineering and Applied Sciences, 11(11), 6779-6793.
[9]. Giwa, A. (2012). Steady-state modeling of n-butyl acetate transesterification process using Aspen Plus: conventional versus integrated, ARPN Journal of Engineering and Applied Sciences, 7(12), 1555-1564.
[10]. Giwa, A. (2013). Methyl acetate reactive distillation process modeling, simulation and optimization using Aspen Plus, ARPN Journal of Engineering and Applied Sciences, 8(5), 386-392.
[11]. Giwa, S.O., Giwa, A. and Hapoglu, H. (2013). Investigating the effects of some parameters on hydrogen sulphide stripping column using Aspen HYSYS. ARPN Journal of Engineering and Applied Sciences, 8(5), 338-347.
[12]. Giwa, A. and Ogunware, M.A. (2018). Modelling, simulation and control of a reactive distillation process for biodiesel production. ABUAD Journal of Engineering Research and Development, 1(1), 49-60.
[13]. Giwa, A., Bello, A. and Giwa, S.O. (2014). Performance analyses of fatty acids in reactive distillation process for biodiesel production. International Journal of Scientific & Engineering Research, 5(12), 529-540.
[14]. Giwa, A., Bello, A. and Giwa, S.O. (2015). Artificial neural network modeling of a reactive distillation process for biodiesel production. International Journal of Scientific & Engineering Research, 6(1), 1175- 1191.
[15]. Giwa, A., Giwa, S.O. and Olugbade, E.A. (2018). Application of Aspen HYSYS process simulator in green energy revolution: a case study of biodiesel production. ARPN Journal of Engineering and Applied Sciences, 13(2), 569-581.
[16]. Giwa, A. and Karacan, S. (2012). Simulation and optimization of ethyl acetate reactive packed distillation process using Aspen Hysys, The Online Journal of Science and Technology, 2(2), 57-63.
[17]. Giwa, A. and Karacan, S. (2012). Nonlinear black-box modeling of a reactive distillation process. International Journal of Engineering Research & Technology, 1(7), 548-557.
[18]. Giwa, A. and Karacan, S. (2012). Decoupling control of a reactive distillation process using Tyreus-Luyben technique. ARPN Journal of Engineering and Applied Sciences, 7(10), 1263-1272.
[19]. Giwa, A. and Giwa, S.O. (2013). Isopropyl myristate production process optimization using response surface methodology and MATLAB. International Journal of Engineering Research & Technology, 2(1), 853-862.
[20]. Giwa, A. and Giwa, S.O. (2013) Estimating the optimum operating parameters of olefin metathesis reactive distillation process. ARPN Journal of Engineering and Applied Sciences, 8(8), 614-624.
[21]. Giwa, A. Giwa, S.O., Bayram, I. and Karacan, S. (2013). Simulations and economic analyses of ethyl acetate productions by conventional and reactive distillation processes using Aspen Plus. International Journal of Engineering Research & Technology, 2(8), 594-605.
[22]. Giwa, A. (2014) Solving the dynamic models of reactive packed distillation process using difference formula approaches. ARPN Journal of Engineering and Applied Sciences, 9(2), 98-108.
[23]. Giwa, A. (2018). Monothetic Analysis of octene metathesis reactive distillation process. ARPN Journal of Engineering and Applied Sciences, 13(4), 1251-1264.

[24]. Giwa, A. and Karacan, S. (2012). Modeling and simulation of a reactive packed distillation column using delayed neural networks. Chaotic Modeling and Simulation, 2(1), 101-108.
[25]. Giwa, A. and Giwa, S.O. (2013). Layer-recurrent neural network modelling of reactive distillation process. Chaotic Modeling and Simulation, 2(4), 647-656.
[26]. Giwa, S.O., Adeyi, A.A. and Giwa, A. (2016). Application of model predictive control to renewable energy development via reactive distillation process. International Journal of Engineering Research in Africa, 27, 95-110.

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