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Prediction for Hydrolysisof Ethylene Oxide via Fuzzy Logic and PID Control

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ABSTRACT

Monoethylene glycol (MEG) or Ethylene Oxide is an important chemical in plastic and automotive industry as mixed ingredients or coolingliquid. It is produced from ethylene oxide via hydrolysis at 200ºC and 22 atm. The ratio of the ethylene oxide withwater should be maintain at 1:20 to reduce the formation of diethylene glycol and higher homologs. Objective of this study is to predict a production of MEG using fuzzy logic. Others parameters such as level, temperature, composition and pressure are consider constant in this research as this study focusing on single input, single (SISO) output strategy. For fuzzy logic prediction, the type of model chosen is Mamdani with triangular membership function, input 1, input 2, and output which refer to error, feedback, and production of ethylene glycol respectively. 11 rules has been construct in this research. The rules may contain "AND" or "OR" conjunctions. The "error" represents the difference between the value feedback and the output. The results for fuzzy rules give highest product of MEG (6.91) at error of 0.102 and 0.8 of feedback. The gain of proportional, integral, and derivative are 0.2, 0.2, and 0.1 respectively.

Keywords: Fuzzy logic, MATLAB, MEG, Prediction

INTRODUCTION

Monoethylene glycol (MEG) is also known as ethylene glycol or 1,2-ethanadiol. MEG is a non - viscous alcohol that are colourless, odourless, and non -volatile (Paiva et al. 2021). It is used as a blending material in polyester fibre and polyethylene terephthalate, which then processed into bottles, cloths, and packaging containers. MEGis also used as an antifreeze medium in heating and cooling systems, hydraulic brake fluid, printer ink, stamp pad ink, and ink for ballpoint pens (Verruschi 2010; National Center for Biotechnology Information 2021).

In a conventional process of producing monoethylene glycol, fossil fuel was used as the rawmaterial that undergo pyrolysis in synthesizing ethylene. Ethylene will be converted into a side product called ethylene oxide via oxidation (Chemical engineering 2015; Priya et al. 2021). Ethylene oxide are easily volatile and undergoes hydrolysis process to produce monoethylene glycol. In the hydrolysis step, anotherseries of steps are presence which are reacting two chemicals, dehydrating, and separating the desired product (Dye et al. 2001) as shown in FIGURE 1.

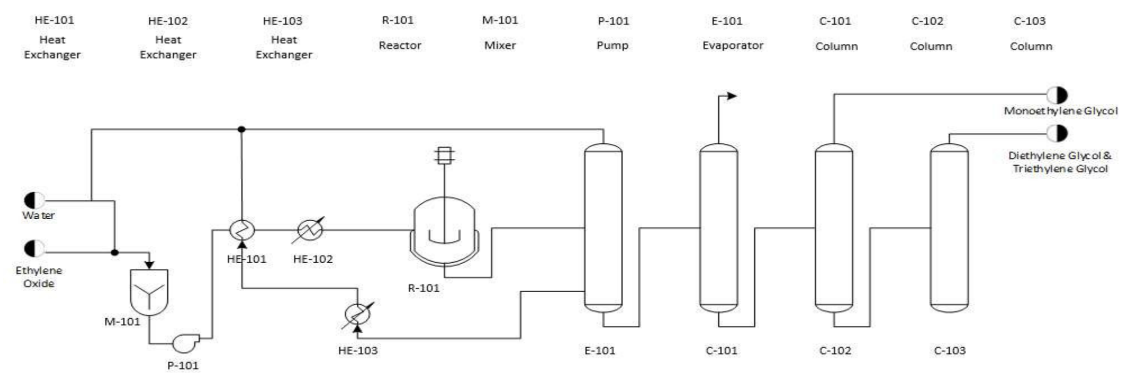

FIGURE 1. PFD of hydrolysis of ethylene oxide

Two chemicals of water and ethylene oxideare reacted with ratio of 20:1 (Harmsen & Verkerk 2020; Kawabe et al. 2010). Both liquids are preheated to 200ºC and pressurized up to 22 atm prior to the stir tank (Akpa et al. 2019). The process follows by boiling the mixture via evaporator before being separated in the next columns.

Other than achieving 80 to 90 percent of conversion via conventional control, large water ratio used inreaction step is an important variable that should be controlled in order to avoid or minimize the production of side product of diethylene glycol (DEG) and Triethylene glycol (TEG) (Dye 2001; Harmsen & Verkerk 2020).

However, at the end of hydrolysis process, it requires removal of excess water that are energy extensive and high operation cost. Dye and members (2001) said that water solely affect the process, not the temperature and pH. Mayer also support the statement where the water plays a major role while both pH and temperature only marginally affect the process of ethylene oxide to monoethylene glycol.

Thus, a good controller should be implemented in order to ensure a high conversion of ethylene oxide to ethylene glycol without producing higher homologues alcohol. The ratio consistency of the water should be taken into account as well. Insteadof using excess water, the hydrolysis process could be improved by using catalyst. Nonetheless, catalyst may also increase the cost as it required separation process and recycle system (Gioacchino et al. 1975).

A conventional control that could be applied to the system for controlling the feed are on-off, P, PI, and PID controller. While theexample of advanced control that can be used is artificial neural network. In this study, the PID andfuzzy logic control will be stimulated to control the feed of the reactor.

IMPLEMENTATION OF PID

PID is the combination of proportional, integral, and derivative control. When there is any change indisturbance, PID will compensate that changes quickly (Omega Engineering, 2019). Commonly the control strategy used with PID is feedback or close loop control strategy (Elprocus 2020). PID controller as shown in FIGURE 2, measures the error that is the differences between current variablevalue and the set point. The compensation is done by forcing the feedback to achieve the set point again until the error is zero or the variable achieve the set point value.

FIGURE 2. PID controller

The tuning strategy of the PID gain value is found by Ziegler & Nichols in 1942 which made it easier. The strategy is applied for a plant that applieda closed controller loop. Firstly, integral and derivative should be set to zero, so that only proportional works alone. The proportional gain should be increased slowly with a small value. The divergence values not allowed. Then, the step change could be performed to observe the response. If it shows a stable oscillation, then the increasing value could be stop and continue with Ki and Kd (Cornejo García 2020).

Proportional, integral, and derivative tuning have different strategy where proportional measure the error and compensate the error. However, it gives a non-steady state condition because there is always error. While I eliminate the error by integrating the error over a period of time but use of integral controller may result a slowprocess because it reduces the output. Decreasing the integral gain may increase the speed response. Lastly, derivative tuning gives more stable system and faster response. It minimizes this overshoot cause by integral tuning by slowing the correction factor applied and compensate it phase lag.

IMPLEMENTATION OF FUZZY LOGIC

Fuzzy logic is one of advance controller that has been develop by Lofti Zadeh in 1965 (Elprocus2020). Fuzzy logic acts similar to how human reasoning and sense. Although there is uncertainties or unclear data, fuzzy convert it into a clear signal (Li et al. 2021; Thakkar et al. 2021) Fuzzy logic works by deciding a list of input and output. The input is commonly represented by A and B, while Zrepresent the product output.

There is a series of step in order to implement fuzzy logic controller as shown in FIGURE 3 below. Firstly, one has to identify the desired control variables to set the membership function. Then list out a minimum and maximumdata value of the inputs and output. These values will be set into 3 range by the tool in MATLAB software.

The steps followed by choosing a fuzzy inferencing system model, either Mamdani orTakagi-Sugeno. A study is done by Mudia (2020) tocompare the performance between of Mamdani-typeand Sugeno-type Fuzzy in controlling the level tank. The modelling of the fuzzy is using the Matlab. Theresult shows Mamdani give a better capability wherethe rise time and the settling time of the response is faster than the Sugeno-type.

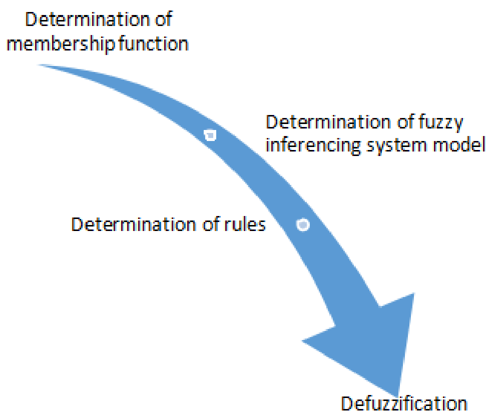

FIGURE 3. Steps of fuzzy logic control

Next, one needs to set the fuzzy tool if-then rules. The rules may contain "AND" or "OR" conjunctions. The rules could be done using expert human logic or by referring past study by other researchers. After the rules setting, one could observe the surface result and rules result as shown in examples of FIGURE 4 and FIGURE 5.

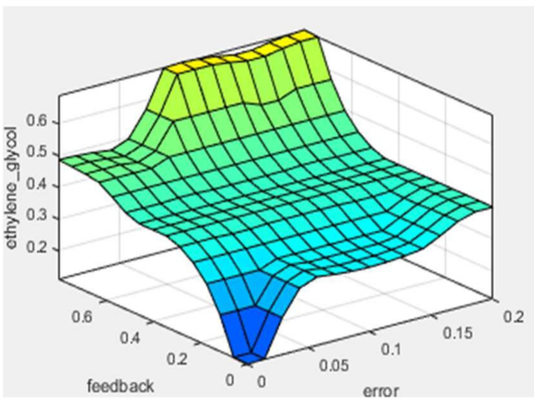

FIGURE 4. Fuzzy surface result

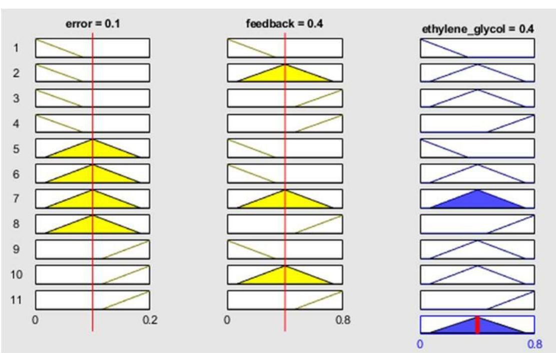

FIGURE 5. Fuzzy rules result

PID controller is widely use in industrial due to ease implementation and can solve many problems. Another advantage is that it can eliminate the steady state error via tuning of integral gain and can estimate future error via derivative action (Ali et al. 2012). PID also require mathematical modelling to develop a transfer function that will use in Matlab/Simulink. However, it is hard to develop a non-linear dynamic process model (Kanthalakshmi 2017).

Fuzzy logic depends on the rules set by human, thus it may be difference for each person. The difference could be minimized when the expertin the process done or by referring past study. According to Goudaet al. (2020), developing fuzzy logic controller is easier and cheaper than PID controller. On top of that, fuzzy has a wider operation range.

SAFETY OF CONTROLLER

Instead of the aim to provide optimum yield at optimum process, installing a controller is also to ensure the safety of the operator and surrounding people. However, a controller always has their disadvantages. A well-known problem associated with PID control is it can overshoot over the desired set point (Ariss & Rabat 2019).The overshoot may affect the standard of the product. The substandard or rejected product will increase the cost of company due to reprocess or disposal activity. In the other hand, overshooting may cause serious incident if the temperature is too high and causing bioreactor explosion. According Ariss & Rabat (2019), the mean square error (MSE) of PID control is increasing if the noise is present.

While, fuzzy logic control also had some issues regarding the safety. According to Markowski et al. (2009) fuzzy control works with uncertainty, it may produceimprecise result. This imprecise result may affect the process and safety as well. Objective of this study are to predict the production of MEG using Fuzzy logic and to evaluate performance of a PID control in term of controlling the feed of the reactor. Others parameters such as level, temperature, composition and pressure are consider constant in this research as this study focusing on single input, single (SISO) output strategy.

METHODOLOGY

CONTROL STRATEGY

Feedback control strategy as shown in FIGURE 6 is used in this study. The sensor detects the changes on the process and send signal to the comparator. The comparator then measured the differences between set point and measured output. An action will be taken by the controller towards the process. The controller could be PID or Fuzzy Logic controller.

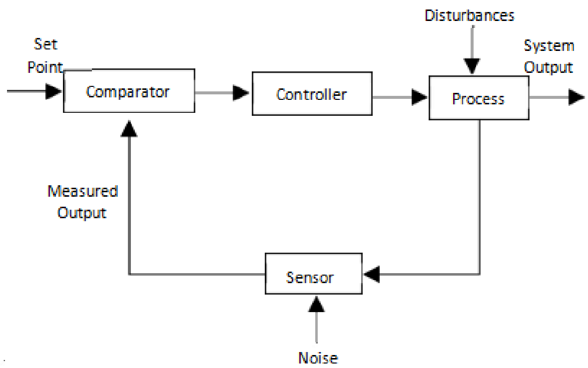

FIGURE 6 Schematic diagram of feedback control
Source: del Giudice 2015; Padhee 2015

CONVENTIONAL CONTROLLER

In this CSTR, two chemicals denoted by X (water) and Y (ethylene oxide) are reacted to produced ethylene glycol that is denoted by Z. In order to develop a transfer function model, a few assumptions (Bourgeois et al. 2006; E.seborg et al. 2004; Stephanopoulos 1984) have been made as listed below:

1. The chemicals are perfectly mixed
2. The heat is negligible in this process
3. The speed of stirring is constant
4. The volume of CSTR is constant

Thus, the total mass balanced for this reaction is:

$$X+Y=Z \tag{1}$$

Then, component mass balance is developed for X and Z as shown in equation 2 and 3 below:

$$\frac{dVC_x}{dt} = F_i C_{x_i} - FC_x + V_{r_x} \tag{2}$$

$$\frac{dVC_x}{dt} = FC_{x_z} + V_{r_x} \tag{3}$$

Where,

C_x is molar concentration of X
C_z is molar concentration of Z
r_x is generation of species X
r_z is generation of species Y

By referring to the study by Aslam & Kaur (2011), the reaction rate is in second order as the water concentration change against the concentration of ethylene oxide, thus the reaction rate for species X and Z as below;

$$r_x = -k_1 C_x - k_3 C_x^2 \tag{4}$$

$$r_Z = k_1 C_X - k_3 C_Z \tag{5}$$

By rearranging equation (2) and combine with equation (4);

$$\frac{dC_x}{dt} = \frac{F_i}{V}(C_{x_i} - C_x) - k_1 C_x - k_3 C_x^2 \tag{6}$$

$$\frac{dC_x}{dt} = \frac{F}{V} C_{x_z} - k_1 C_x - k_3 C_z \tag{7}$$

Both equation (6) and (7) are applied into state space model.

$$A = \begin{bmatrix} \frac{F_s}{V} - k_1 C_x - k_3 C_x^2 & 0 \\ k_1 & -\frac{F_s}{V} - k_2 \end{bmatrix}$$

$$B = \begin{bmatrix} C_{xf_s} - C_{x_s} & \frac{F_s}{V} \\ C_{z_s} & 0 \end{bmatrix}$$

Based on Aslam and Kaur (2011), the values for k_1, k_2, k_3, C_{xs}, C_{zs}, and $\frac{Fs}{V}$ are as follow;

$k_1 = 0.8333\text{min}$
$k_2 = 1.6667\text{min}$
$k_3 = 0.1667\text{min}$
$C_{xs} = 3$ gmol/liter
$C_{zs} = 1.117$ gmol/liter
$C_{xf_s} = 10$ gmol/liter
$\frac{Fs}{V} = 0.5714\text{min}^{-1}$

After substitute all the value, the space state model is as follow;

$$A = \begin{bmatrix} -2.4048 & 0 \\ 0.8333 & -2.2381 \end{bmatrix}$$

$$B = \begin{bmatrix} -7 & 0.5714 \\ -1.117 & 0 \end{bmatrix}$$

$$C = \begin{bmatrix} 0 & 1 \end{bmatrix}$$

$$D = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

Thus, the transfer function given by MATLAB is:

$$G_p(s) = \frac{-1.1117s + 3.1472}{s^2 + 4.6429s + 5.3821}$$

The transfer function was then applied in MATLAB/SIMULINK. FIGURE 7 shows the modelling of system without PID control.

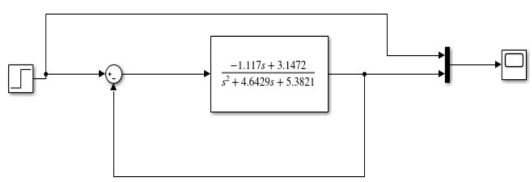

FIGURE 7. Process modelling in Matlab/Simulink

The system with PID controller is shown in FIGURE 8. The gain of proportional, integral, and derivative are 0.2, 0.2, and 0.1 respectively. The tuning is done by using Ziegler & Nichols method.

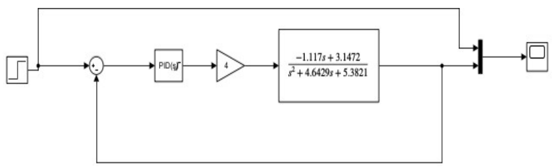

FIGURE 8. Process modelling with PID control in Matlab/Simulink

FUZZY LOGIC

A fuzzy tool was used in MATLAB to be stimulate in MATLAB/SIMULINK. By typing “fuzzy” in MATLAB command window, a fuzzy tool will come out. Every setting including type of model, membership function, and rules should be set according to desired system.

Firstly, the type of model chosen are Mamdani. Then the membership function is filled in for input 1, input 2, and output which refer to error, feedback, and production of ethylene glycol respectively. The “error” represents the difference between the value feedback and the output.

A range of data values were set for each ofthem where input 1 is [0 0.2], input 2 is [0 0.8], output is [0 0.8]. It was estimate that 80% of ethylene oxide will be converted to ethylene glycol.The values for each membership function was set forminimum, medium, and maximum values by the tool based on the range applied as shown in Figure 9, Figure 10 and Figure 11.

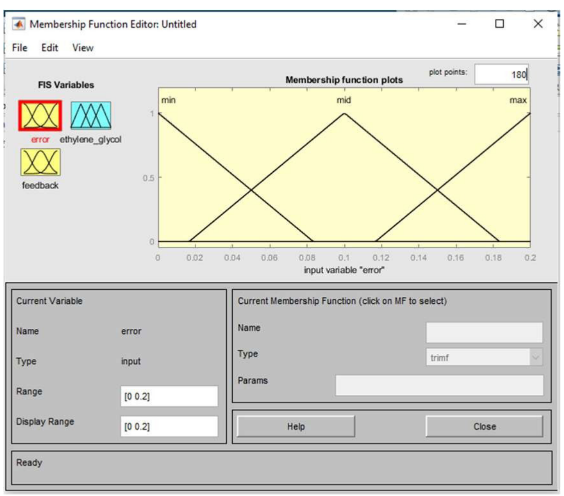

FIGURE 9. Membership function for input 1 (error)

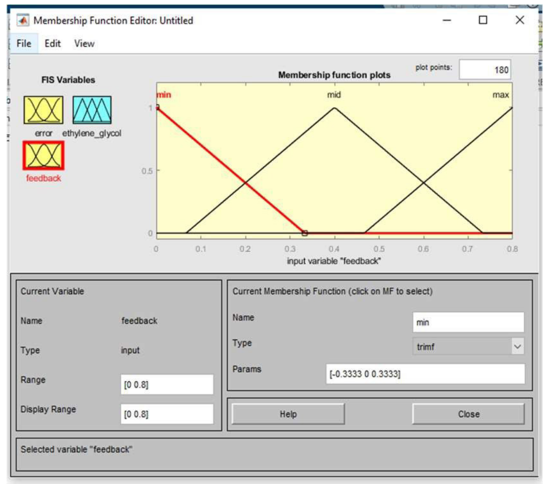

FIGURE 10. Membership function for input 2 (feedback)

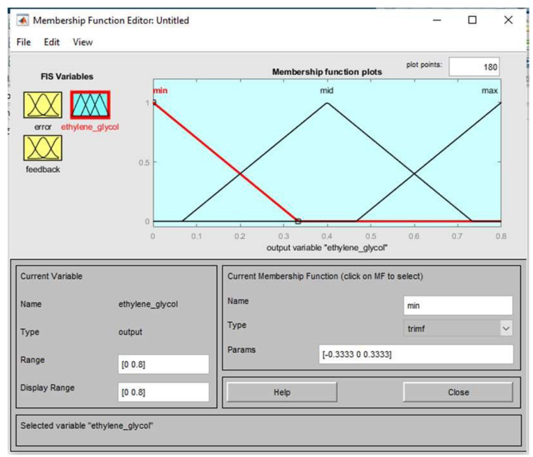

FIGURE 11. Membership function for output (ethyleneglycol)

Then, “if-then” rules have been added intothe fuzzy tool system. The 11 rules using “and” conjunctions are shown in Figure 12.

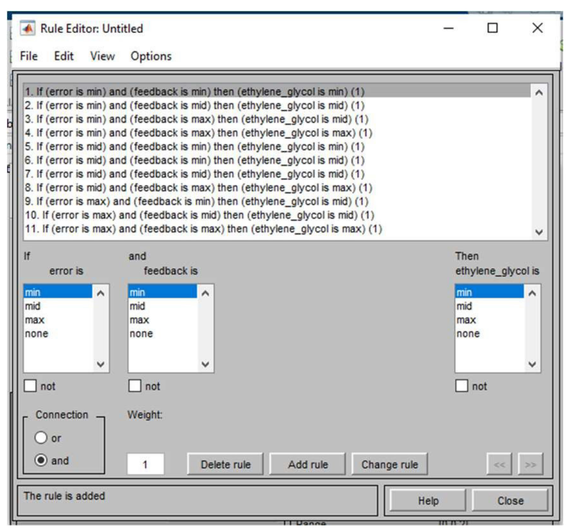

FIGURE 12. Rules of fuzzy tool

Then, the result of fuzzy tool will be submerged to the fuzzy model in Matlab/Simulink. The modelling of fuzzy control is shown by Figure 13 below.

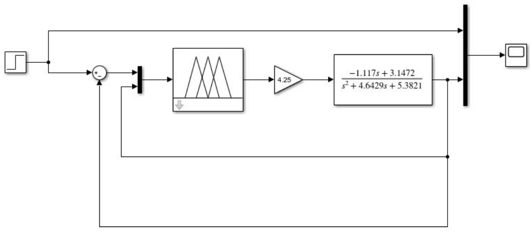

FIGURE 13. Modelling of fuzzy control in Matlab/Simulink

RESULT AND DISCUSSION

CONVENTIONAL CONTROLLER

Figure 14 shows the graph without PID controller. The system with transfer function applied (red line)shows a steady state at around 0.35 second. There isalso offset at early period of time.

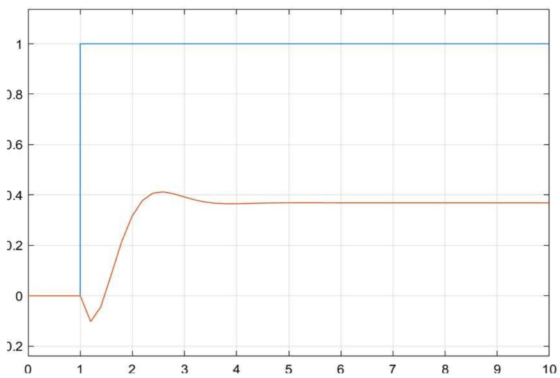

FIGURE 14 Model system response without PID control

Figure 15 indicate the result (red line) ofPID tuning. The steady state is achieved at 10 seconds which is much slower than the system without controller. While the rise time of the response is at 3.9 seconds. The response of PID control also give higher overshoot percentage whichis 0.631% compare to without controller (0.505%).

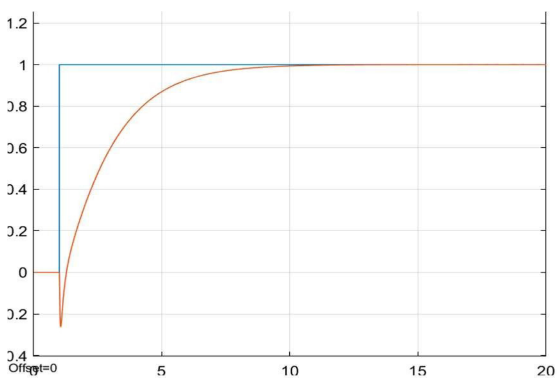

FIGURE 15. System response with PID controller

FUZZY LOGIC PREDICTION

Figure 16 is the result for each rules for the prediction of MEG/ ethylene glycol using fuzzy logic. The results in general similar with the Vitiyah et al. (2020) with different in terms of inputs and output.

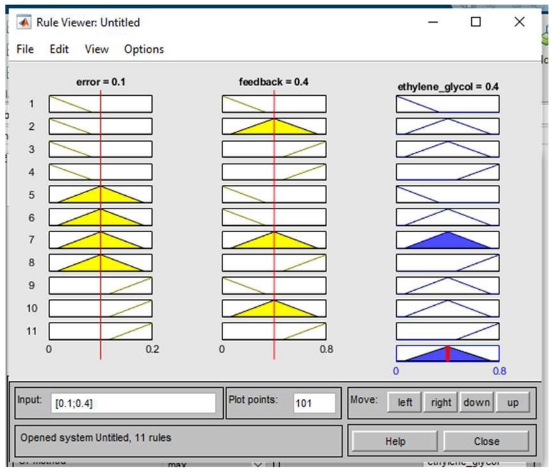

FIGURE 16. Fuzzy rules result

At the mid line of the input rules, the outputof ethylene glycol gives 0.4. By referring Figure 17, the input of error is at median (0.102) while input feedback at the maximum (0.8) which also gave highest conversion of ethylene oxide to monoethylene glycol up to 6.91.

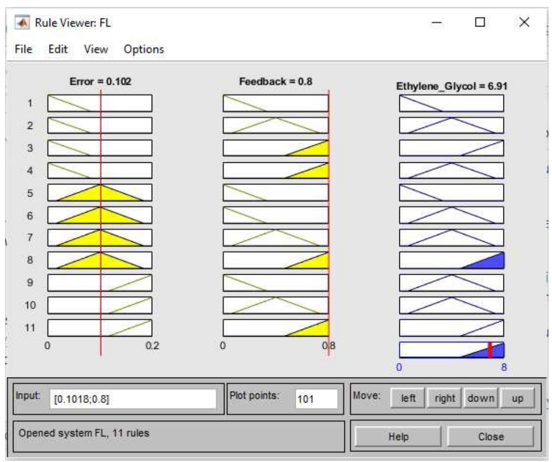

FIGURE 17. Fuzzy rules result (highest output)

Both rules and surface result were load into Matlab/ Simulink fuzzy model. The result may beerror due to setting and transfer function as the process quite similar with study by Vitiyah et al. (2020) and Nur Najihah et al. (2018).

CONCLUSION

Performance for both control system did not show a good result. This is probably due to incorrect mathematical modelling orthe Matlab/ Simulink setting. Instead of 0 result of fuzzy control, PID shows a steady state control at 1 with earlier rise time of 3.9 second compared to control system at 5.56 seconds. Generally, PID control could not eliminate the offset and fuzzycontrol is unsuccessful.

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DECLARATION OF COMPETING INTEREST

None

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