IOP Conference Series: Materials Science and Engineering

PAPER • **OPEN ACCESS**

Optimization process for ethylene glycol production using the Pareto solution

To cite this article: M S Sulaiman *et al* 2021 *IOP Conf. Ser.: Mater. Sci. Eng.* **1011** 012003

View the article online for updates and enhancements.

IOP Conf. Series: Materials Science and Engineering 1011 (2021) 012003 doi:10.1088/1757-899X/1011/1/012003

Optimization process for ethylene glycol production using the Pareto solution

M S Sulaiman, F S Rohman S and N Aziz*

School of Chemical Engineering, Engineering Campus, Universiti Sains Malaysia, Seri Ampangan, 14300 Nibong Tebal, Seberang Perai Selatan, Penang, Malaysia.

*Corresponding author: chnaziz@usm.my

Abstract. In this work, ε-constraint approach within ASPEN Plus environment is used to generate the Pareto solutions for two objectives: maximize productivity and minimize energy consumption, for the ethylene glycol production. Each point of Pareto solutions consists of different optimal temperature and hydrogen flowrate values, which lead to distinct amount of energy consumption and ethylene glycol product rate. These solutions give flexibility in evaluating the trade-offs and selecting the most suitable operating policy. The most satisfactory optimum and trade-off of both objectives is determined. The optimum value for ethylene glycol production and energy consumption are 109.92 kmol/hr and 11227860.10 kJ/hr, respectively, while the trade-off values are 18.02 kmol/hr and 10903846.2 kJ/hr, respectively. The comparison between multi-objective optimization and single-objective optimization concludes that a high benefit against disadvantages is achieved by implementing multi-objective optimization. The difference between multi-objective optimization and single-objective optimization for ethylene glycol production and energy consumption are –5.65 kmol/hr and 17526931.8 kJ/hr, respectively.

1. Introduction

Production of EG is rapidly increasing and is predicted that this increment will continue until 2030 [1]. EG is used as raw materials in the production of a wide range of products including polyester fibers, fiberglass and polyethylene terephthalate [2]. Industries involved in the production of EG have their own methods and approaches in attaining their target (high production rate or cost saving). Most of these techniques involved optimization of certain objectives.

Optimization is to make the best or most effective use of a situation or resource. Referring to this statement, the production of EG requires optimization for; energy consumption reduction, maximizing productivity, reduction of side products, minimizing feed requirements etc. These objectives usually conflict with one another and thus most industries prioritized only one resulting in inefficient plant operations. In the EG process, there are conflicting objective functions, i.e. maximum production and minimum energy consumption which cannot be solved by single objective optimization technique. Simultaneous optimization of these objectives yields in a MOO problem, which is characterized by a set of multiple solutions, known as Pareto solutions.

MOO is defined as an area of multiple criteria decision making that is concerned with mathematical optimization problems involving more than one objective function to be optimized simultaneously where optimal decisions need to be taken in the presence of trade-offs between two or more conflicting objectives. For a nontrivial MOO problem, no single solution exists that simultaneously optimizes each objective. In that case, the objective functions are said to be conflicting, and there exists a (possibly

IOP Conf. Series: Materials Science and Engineering 1011 (2021) 012003 doi:10.1088/1757-899X/1011/1/012003

infinite) number of Pareto optimal solutions. A solution is called Pareto optimal, if none of the objective functions can be improved in value without degrading some of the other objective values. Different solution philosophies and goals are developed when setting and solving MOO problems due to the difference in points of views [3].

Pareto (optimal) solutions are range of solutions (objectives) used in acquiring the Pareto optimal set. Pareto optimal set is a set of all the solutions located in the feasible decision space. The boundary defined by the set of all point mapped from the Pareto optimal set is called the Pareto optimal front. Pareto optimal solutions are obtained through various applicable methods such as ε-Constraint Method - Keep just one of the objective and restricting the rest of the objectives within user-specific values, Weighted Sum Method - Scalarize a set of objectives into a single objective by adding each objective pre-multiplied by a user-supplied weight and Weighted Matrix Method - Combine multiple objectives using the weighted distance metric of any solution from the ideal solution [4].

MOO has been increasingly employed in chemical engineering and manufacturing. An optimization of the pressure swing adsorption process (cyclic separation process) involving dual maximization of nitrogen recovery and nitrogen purity using the multi-objective genetic algorithm (MOGA) was developed by Fiandaca and Fraga in 2009. A fine approximation of the Pareto frontier with acceptable trade-offs between the objectives results was produced [5]. In 2010, a multi-objective problem for the thermal processing of food involving two case studies (bi-objective and triple objective problems) with nonlinear dynamic models were solved by Sendín *et al.* using a hybrid approach consisting of the weighted Tchebycheff and the Normal Boundary Intersection approach [6].

A MOO of the combined carbon dioxide reforming and partial-oxidation of methane involving the objective functions of methane conversion, carbon monoxide selectivity and hydrogen to carbon monoxide ratio were performed by Ganesan *et al.* using the Normal Boundary Intersection (NBI) method in conjunction with two swarm-based techniques (Gravitational Search Algorithm (GSA) and Particle Swarm Optimization (PSO)) in 2013[7]. In the same year, an alternative technique to solve multi-objective optimization problems using the Aggregating Functions Approach, the Adaptive Random Search Algorithm, and the Penalty Functions Approach were used to compute the initial set of the non-dominated or Pareto-optimal solutions were proposed by Abakarov *et al.* [8]. In 2018, an approach using a Mixed-Integer Linear Program to solve the optimization problem for a weighted sum of the two objectives to calculate a set of Pareto optimal solutions were formulated by Pearce *et al.* The application of the approach showed improvements in at least one objective in most tasks and in both objectives in some of the processes [9].

Based on previous researches, various MOO techniques have been implemented to different kinds of processes. However, it is comprehended that the Single Objective Optimization (SOO) is used in the production of EG. This hinders the process to operate at its best optimal condition as SOO can mitigate only one objective. Thus, this research fills the gap by implementing MOO for the production of EG to maximize productivity and minimizing energy consumption simultaneously.

2. Methodology

2.1. Modelling and Initial Optimization

A reactor model is taken from Yu and Chien (2017) and simulated using ASPEN Plus V11 [10]. The model is constructed as in figure 1. It is a Plug Flow Reactor (PFR) model which comprises the characteristics stated in table 1.

IOP Conf. Series: Materials Science and Engineering 1011 (2021) 012003 doi:10.1088/1757-899X/1011/1/012003

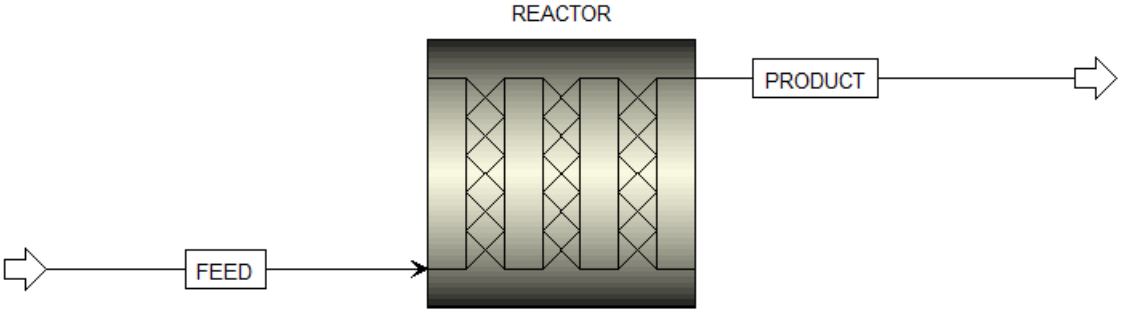

Figure 1. ASPEN Plus Plug Flow Reactor model.

Table 1. Specification of ASPEN Plus PFR model.

Feed Parameter	Quantity	Reactor Parameter	Quantity
Temperature	160 ºC	Temperature	210 ºC
Pressure	25 bar	Pressure	25 bar
Mole Flow	7059.97 kmol/hr	Length	5 m
DMO	0.0179072 %	Diameter	1 m
MEOH	0.264306 %	Bed Voidage	0.5
MG	0.0005002 %	Particle Density	980 kg/cum
H_2	0.717187 %		
CO	0.00010004 %		

The model is then optimized to increase the production of EG by obtaining the highest possible yield. This optimization refers to SOO. The purpose of this optimization is compared (benchmarking) with MOO. First, all related inputs and outputs are defined. The objective is set to attain maximum yield. There are no constraints applied to the optimization process. Feed hydrogen and reactor temperature is set as the manipulated variable (MV). The executable statement for the process is set as shown in Equation 1.

2.2. Correlation of Objectives

The objectives of MOO are determined which are EG production and energy consumption. The corresponding equations relating both objectives are constructed as shown equation 1 to 6.

$$a = (DMO\ IN \cdot 65.57 + MEOH\ IN \cdot 31.63 + MG\ IN \cdot 129.32 + H2\ IN \cdot 28.24 + CO\ IN \cdot 29.15)(TOUT - T\ IN) \quad (1)$$

$$b = (DMO\ IN \cdot 65.57 + MEOH\ IN \cdot 31.63 + MG\ IN \cdot 129.32 + H2\ IN \cdot 28.24 + CO\ IN \cdot 29.15)(25 - T\ IN) \quad (2)$$

$$c = (EG\ OUT \cdot 162.5 + ETOH\ OUT \cdot 209.9 - DMO\ IN \cdot 372.8) \quad (3)$$

$$d = (DMO\ OUT \cdot 65.57 + MEOH\ OUT \cdot 31.63 + MG\ OUT \cdot 129.32 + H2\ OUT \cdot 28.24 + CO\ OUT \cdot 29.15 + EG\ OUT \cdot 77.99 + ETOH\ OUT \cdot 65.21 + H20\ OUT \cdot 33.59)(T\ OUT - 25) \quad (4)$$

$$e = (111.7 + 77.99(T\ OUT - 25) \quad (5)$$

$$EG\ OUT = (a + b + c + d) \cdot e^{-1} \quad (6)$$

2.3. Optimization

For the ASPEN Plus optimization process, three separated simulation is carried out relating EG production to energy consumption which are Low Energy (LE) optimization, High Product (HP) optimization and MOO. LE and HP Optimization is to determine the boundary of the Pareto optimal front.

2.3.1. LE and HP Optimization. For HP optimization, the objective is set to gain maximum product. All related inputs and outputs required for the process are defined. There are no constraints applied to the optimization process. Feed hydrogen and reactor temperature is set as the manipulated variable (MV). The executable statement for the process is set as shown in Equation 1. As for LE optimization, the objective is set to gain minimum energy consumption. All related inputs and outputs required, constraints and MV are the same as HP optimization. The executable statement for the process is set as shown in equation 1.

2.3.2. MOO. For MOO, the steps are the same as HP optimization. However, there are constraints added to the optimization process. These constraints (EGOUT and Q) are obtained and defined based on the ε-constraint method. The ε-constraint method is stated in equation 7.

$$minimize\ f_\mu(x),$$

$$subject\ to\ f_m(x) \leq \varepsilon_m, m = 1, 2, \dots, M\ and\ m \neq \mu$$

$$g_j(x) \geq 0, j = 1, 2, \dots, J$$

$$h_k(x) = 0, k = 1, 2, \dots, K$$

$$x_i^{(L)} \leq x_i \leq x_i^{(U)}, i = 1, 2, \dots, n \tag{7}$$

2.4. Pareto Chart

The Pareto front is plotted using the result obtained from the MOO section. The relationship between objectives, between MVs and between objectives and MVs are studied and discussed. The optimum values for EG production and energy consumption are determined. Comparison of MOO and SOO are made.

3. Result and Discussion

The reactor model was validated by experimental data from Li *et al.* (2015) [11] and Yu and Chien (2017) [10].

3.1. Objective Optimization

In order to optimize the objectives, it is first required to understand the characteristic of the respective objectives with changes in MVs. Figure 2, 3, 4 and 5 displays the characteristic of individual objectives against MV. Objective 1 represents product flow (EG), objective 2 represents energy consumption (Q), MV1 represents hydrogen flowrate and MV2 represents temperature. Hydrogen flowrate and temperature is chosen as the MVs because they are the factors directly affecting the rate of reaction [12].

From figure 2, it shows a nonlinear curve of which objective 1 increase as MV1 increase. The increment reduces as objective 1 reaches its maximum point. The slow increase is caused by maximum reaction rate limit. In other words, the production of EG is at its highest due to the rate of reaction reaching its maximum point. This is in line with the reaction rate and kinetic [10]. Thus, the EG production rate cannot be further increased.

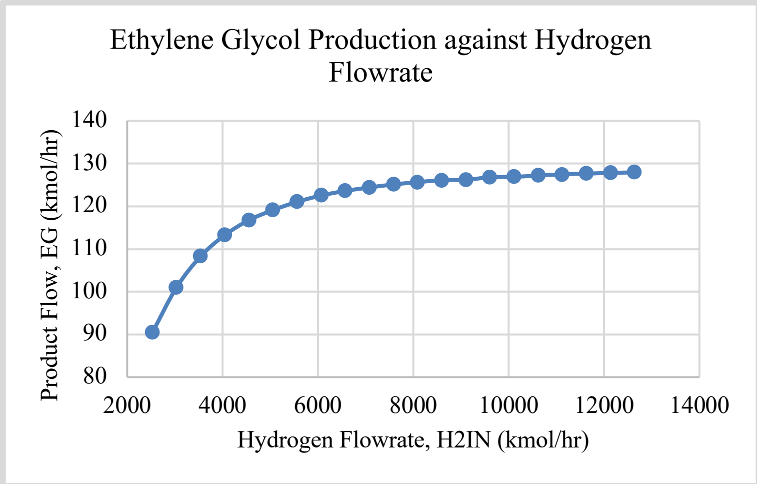

Figure 2. Relationship of MV1 and Objective 1.

Figure 3 shows that objective 1 increase exponentially as MV2 increase. However, objective 1 suffers steady fall once MV2 rises beyond 194 °C. This is due to more side products are formed as the reactor temperature increases. A chain reaction causing the rise in formation of side product due to more main product being consumed explains the fall of objective 1. This follows the Le Chatelier's principle [13].

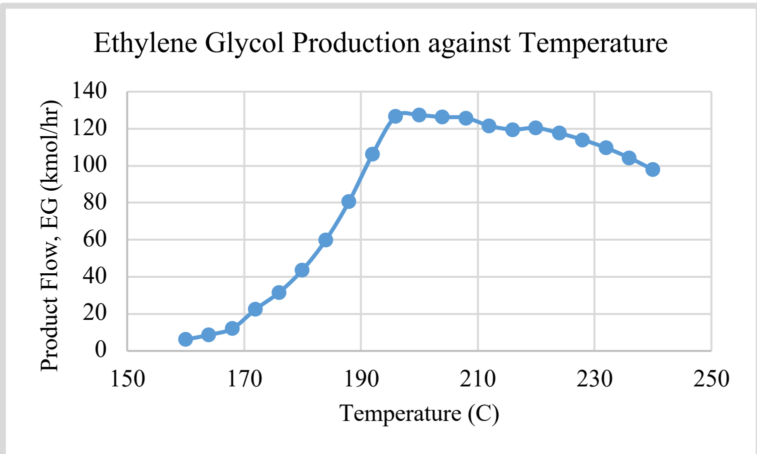

Figure 3. Relationship of MV2 and Objective 1.

From figure 4, it is seen that the graph has an almost linear increment. This shows that as MV1 rise, objective 2 increases. Since the reaction is exothermic, this leads to more energy released with increasing reaction thus, obeys the law of thermodynamics [14]. With higher hydrogen flowrate, lower energy consumption is achieved.

Figure 5 shows that as MV2 rise, objective 2 increases. This increment however continues with a fall. This is due to at first low temperature is used, so the energy released from the exothermic reaction helps in providing additional energy [14]. But as the temperature increases, more energy is required to heat up the reactor causing the rise in energy consumption.

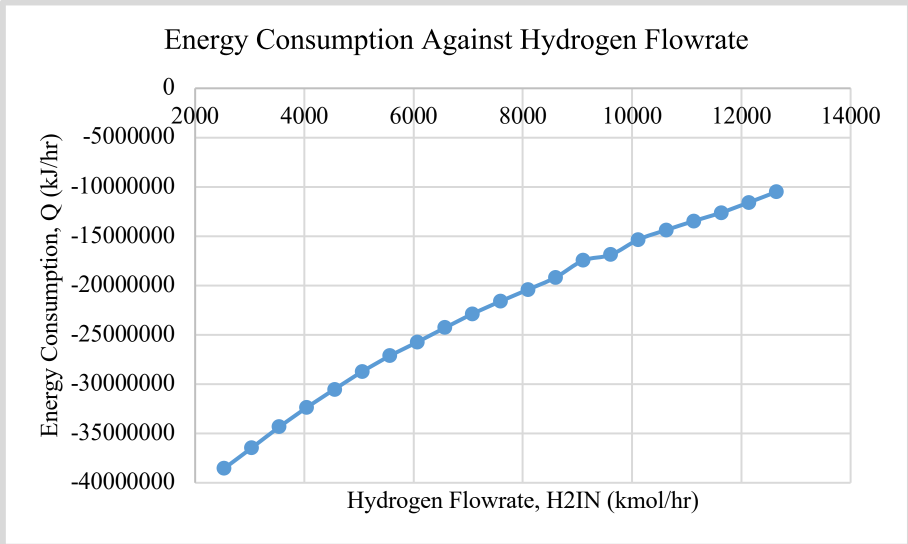

Figure 4. Relationship of MV1 and Objective 2.

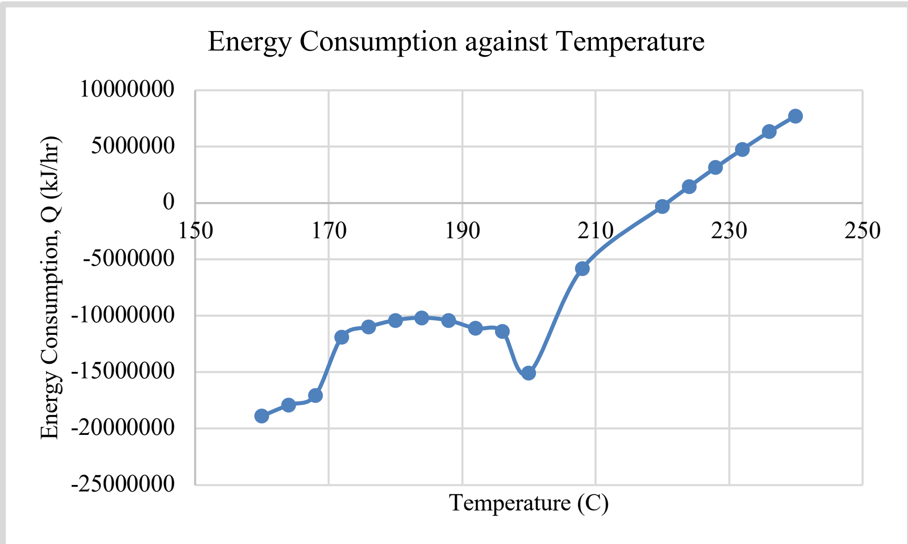

Figure 5. Relationship of MV2 and Objective 2.

To achieve a fine MOO, the hydrogen flowrate must be high for better EG production and lower energy consumption. The temperature must be strictly controlled in order to determine the best EG production while maintaining low energy consumption.

3.2. Multi-Objective Optimization

ε-constraint method is selected because it is applicable to either convex or non-convex problems [15]. That makes it perfect for this case since no solid grasp on the Pareto foundation can be made at this point. In addition, the method is thoroughly simple except in determining the epsilon (multi-objective) range. The range must fulfilled the requirements in which the objectives have to be within the range. This is the reason for the LE and HP optimizations. With the optimizations data, a range (constraints) for the objectives is developed as shown in equation 8.

$$max\ f_{EG}(x);\ f_Q = -24900468.30 \ll \varepsilon$$

$$f_{EG} = 127.93 \gg \varepsilon$$
$$\min f_Q(x);\ \ f_{EG} = 7.81 \gg \varepsilon$$
$$f_Q = -324013.90 \ll \varepsilon$$
$$-24900468.30 \ll \varepsilon \ll 127.93 \tag{8}$$

The constraints are manipulated within the range and a set of data are obtained. A Pareto front is plotted for production of EG against energy consumption. The purposed of the plot is to identify the optimum point which satisfied both objectives accordingly.

From figure 6, an inverse s-curved plot is obtained. A point named Utopia point is marked on the plot. The Utopia point is the ideal point in which is the ideal values for each objective. This point serves as a reference point in regards of finding the actual optimum point [16]. Thus, point B which is the true optimum point (value) is acquired. Point B is selected as the optimum point because it has the shortest distance with the Utopia point which justified that point B is the nearest to ideal-optimum value. From the plot, the trade-off between both objectives is also known. This shows that indeed both the objectives are in conflict without dominating each other.

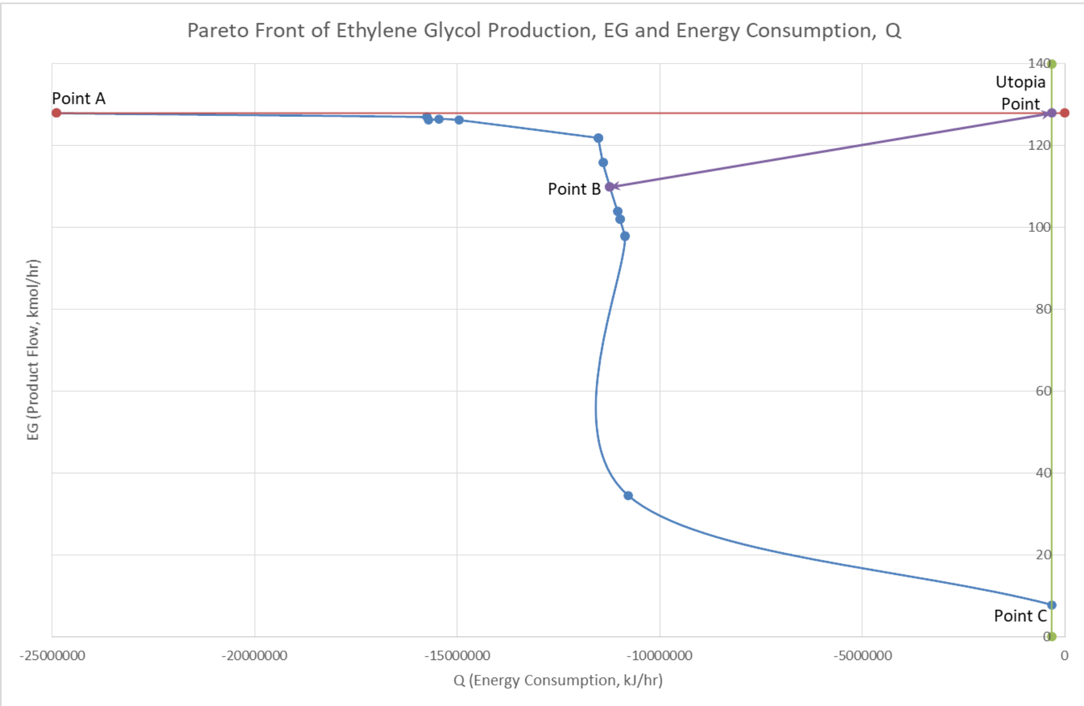

Figure 6. Pareto Optimal Front.

The optimum value for EG production and energy consumption are 109.92 kmol/hr and 11227860.10 kJ/hr, respectively. On the other hand, the trade-off value for EG production and energy consumption are 18.02 kmol/hr and 10903846.2 kJ/hr, respectively.

To further proved that the Pareto front in figure 6 is acceptable, figure 7 is plotted. From the plot, it is observed that MV2 rises with constant MV1. MV1 then decrease drastically once MV2 is beyond 194°C. The MVs for optimum point (Utopia point) is located before 194°C. This corresponds with the objective and MV relationship in figure 2, 3, 4 and 5. Thus, the validity of the Pareto optimal solution is confirmed.

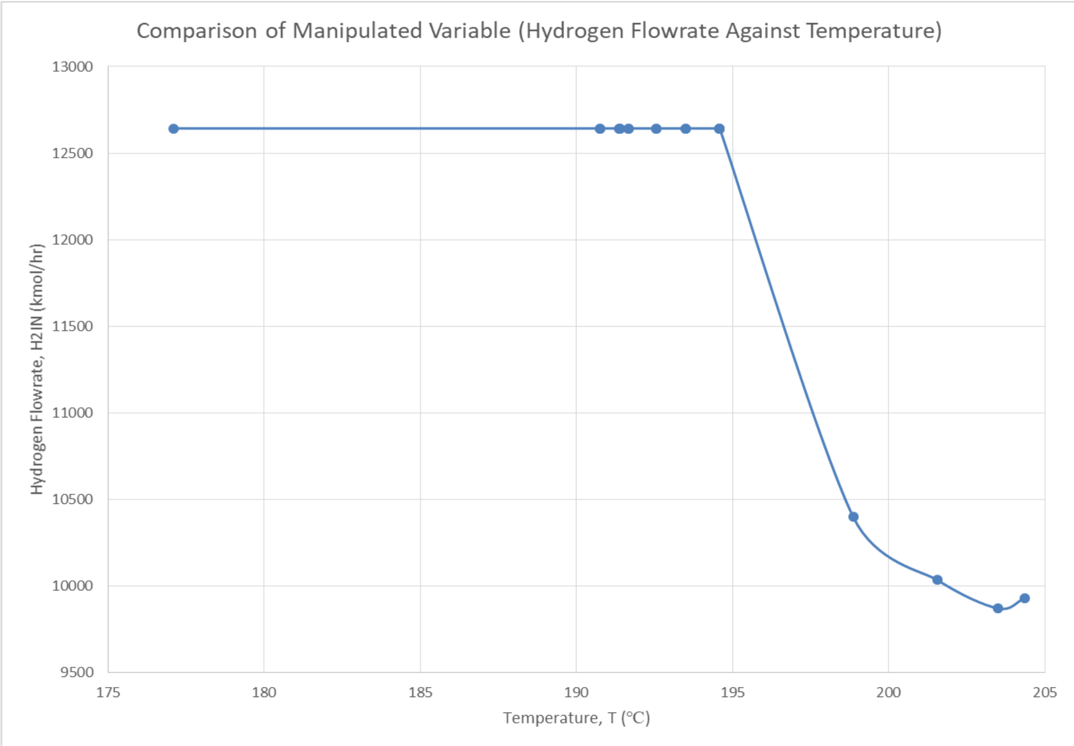

Figure 7. Pareto Optimal Solution.

3.3. Comparison of MOO and SOO
From table 2, it is seen that the production of EG for SOO is higher and with much lower feed hydrogen than MOO. However, the reactor temperature and energy consumption for MOO is lower than SOO. As observed in figure 2, 3, 4 and 5, energy consumption can be reduced by increasing hydrogen flowrate. The difference between MOO and SOO for ethylene glycol production and energy consumption are -5.65 kmol/hr and 17526931.8 kJ/hr, respectively. The difference in energy consumption is large with MOO having lower value and the difference in EG production is relatively small with SOO having higher value.

Table 2. Results for SOO and MOO.

	SOO	MOO	Unit
H2 IN	5063.32	12642.43	kmol/hr
H2 OUT	4574.38	12192.00	kmol/hr
EG OUT	115.57	109.92	kmol/hr
T OUT	210.00	192.56	°C
Q	-28754791.9	-11227860.1	kJ/hr

The decrease in EG production is acceptable because of the high drop in energy consumption which leads to a lower operating temperature creating a safer environment. The increase in hydrogen required is exceptionally high but can be countered by proper recycling of feed. Thus, the overall comparison showed high benefits with slight trade-off.

4. Conclusion
The overall optimization process is a success. A well-developed PFR model served excellently in error prevention. The interaction between MV1 and MV2 with objective 1 and objective 2 is highly dependent. Objective 2 is much more sensitive towards the change in MV1 and MV2 compared to objective 1. The interaction between MV1 and MV2 is unique in which it cannot be seen until 194°C.

The optimum value for EG production and energy consumption are 109.92 kmol/hr and 11227860.10 kJ/hr, respectively while the trade-off values are 18.02 kmol/hr and 10903846.2 kJ/hr, respectively. The difference between MOO and SOO for EG production and energy consumption are -5.65 kmol/hr and 17526931.8 kJ/hr, respectively. This shows that the comparison between MOO and SOO results in objective 1 for SOO is slightly higher than MOO but for objective 2, MOO is significantly higher than SOO. This concludes that a high benefit with slight trade-off (high energy consumption reduction and slight decrease in EG production) is achieved by implementing MOO.

Acknowledgement
The financial support from Universiti Sains Malaysia through Research University Grant (RUI) 203.PJKIMIA.8014146 is greatly acknowledged.

References

[1] American Chemistry Council (ACC) Inc 2020 What is Ethylene Glycol?
[2] Garside M 2019 Global production capacity of ethylene 2018 & 2030
[3] Fiandaca G, Fraga E S and Brandani S 2009 A multi-objective genetic algorithm for the design of pressure swing adsorption *Eng. Optimiz.* **41(9)** 833–54
[4] Deb K 2001 *Multi-Objective Optimization using Evolutionary Algorithms* John Wiley & Sons, Inc 13-80
[5] Rohman F S and Aziz N 2020 Multi-objective optimization of batch electrodialysis for minimizing energy consumption by using non-dominated sorting genetic algorithm (NSGA-II) *IOP Conference Series: Materials Science and Engineering* 736
[6] Sendín J O H, Alonso A A and Banga J R 2010 Efficient and robust multi-objective optimization of food processing: A novel approach with application to thermal sterilization *J. Food Eng.* **98(3)** 317–24
[7] Ganesan T, Elamvazuthi I, Ku Shaari K Z and Vasant P 2013 Swarm intelligence and gravitational search algorithm for multi-objective optimization of synthesis gas production *Applied Energy* **103** 368–74.
[8] Abakarov A, Sushkov Yu and Mascheroni R H 2012 Multi-criteria optimization and decision-making approach for improving of food engineering processes *Int. J. Food Stud.* **2** 1–21
[9] Pearce M, Mutlu B, Shah J and Radwin R 2018 Optimizing Makespan and Ergonomics in Integrating Collaborative Robots into Manufacturing Processes *IEEE T. Autom. Scie. Eng.* **15(4)** 1772–84
[10] Yu B-Y and Chien I L 2017 Design and optimization of dimethyl oxalate (DMO) hydrogenation process to produce ethylene glycol (EG) *Chem. Eng. Res. Des.* **121** 173-90
[11] Li S, Wang Y, Zhang J, Wang S, Xu Y, Zhao Y and Ma X 2015 Kinetics study of hydrogenation of dimethyl oxalate over cu/sio2 catalyst Industrial & Engineering Chemistry Research **54** 1243-50
[12] Tro N J *Chemistry: Structure and Properties, 2nd Edition* Pearson Chapter 14
[13] Knox K 1985 Le Châtelier's Principle *Journal of Chemical Education* **62** 863
[14] Stepanov I A 2000 The 1st Law of Thermodynamics in Chemical Reactions *Chemical Physics*
[15] Rohman F S and Aziz N 2019 Performance metrics analysis of dynamic multi-objective optimization for energy consumption and productivity improvement in batch electrodialysis *Chem. Eng. Commun.* 1-13
[16] Qi Y, Zhang Q, Ma X, Quan Y and Miao Q 2017 Utopian point-based decomposition for multi-objective optimization problems with complicated Pareto fronts *Appl. Soft Comput.* **61** 844-59