SEMARAK ILMU PUBLISHING

Semarak Engineering Journal

Journal homepage:
https://semarakilmu.com/
ISSN: 3036-0145



Optimisation Strategy of Methanol Production Using Swarm Based Techniques

Fakhrony Sholahudin Rohman[1], Mohd Azahar Mohd Ariff[2], Dinie Muhammad[3], Muhamad Nazri Murat[4], Zulkifli Abdul Rashid[5], Iylia Idris[5,6], Dipesh Shikchand Patle[7], Ashraf Azmi[5,6,*]

[1] Faculty of Engineering, Universiti Malaysia Sabah, 88400, Kota Kinabalu, Sabah, Malaysia
[2] Faculty of Chemical Engineering, Universiti Teknologi MARA, Cawangan Pulau Pinang, Kampus Permatang Pauh, 13500 Permatang Pauh, Pulau Pinang, Malaysia
[3] School of Chemical and Energy Engineering, Faculty of Engineering, Universiti Teknologi Malaysia (UTM), Johor Bahru, Johor 81310, Malaysia
[4] School of Chemical Engineering, Engineering Campus, Universiti Sains Malaysia, 14300 Nibong Tebal, Pulau Pinang, Malaysia
[5] Faculty of Chemical Engineering, Universiti Teknologi MARA, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia
[6] Integrated Separation Technology Research Group, Faculty of Chemical Engineering, Universiti Teknologi MARA, 40450, Shah Alam, Selangor, Malaysia
[7] Department of Chemical Engineering Motilal Nehru National Institute of Technology Allahabad, Prayagraj, India-211004

ARTICLE INFO

Article history:
Received 12 February 2026
Received in revised form 21 March 2026
Accepted 18 May 2026
Available online 9 June 2026

Keywords:
Multi-Objective Optimisation (MOO); Methanol; Multi-objective Particle Swarm Optimisation (MOPSO); Multi-objective Dragonfly Algorithm (MODA); Multi-objective Slime Mould Algorithm (MOSMA)

ABSTRACT

Multi-objective optimisation (MOO) of methanol (CH_3OH) production in a fixed-bed catalytic reactor was carried out by considering five objectives: maximising CO_2 conversion (XCO_2) and methanol production rate (FCH_3OH), while minimising bare module cost (CBM), energy cost (CostE), and side product formation (FH_2O). An Aspen Plus simulator was used for the model-based optimisation of the CH_3OH production process. Multi-objective swarm-based optimisation algorithms, namely Multi-objective Particle Swarm Optimisation (MOPSO), Multi-objective Dragonfly Algorithm (MODA) and Multi-objective Slime Mould Algorithm (MOSMA) were integrated with the Aspen simulation model to solve the optimisation problems. The optimisation methods were evaluated using hypervolume, pure diversity, and spacing performance metrics. Based on the results obtained, MOSMA showed better overall performance, with a solution set that demonstrated good convergence, diversity, and distribution along the Pareto Front (PF). Furthermore, the decision variable plots indicate that reactor pressure significantly influenced the optimal solution. The results obtained include a conversion of 0.567, a product rate of 2784.147 kmol/hr, an energy cost of 0.773 Mil. RM/year, a CBM of 0.054 Mil. RM, and a side product formation of 270.399 kmol/hr.

* *Corresponding author.*
E-mail address: ashraf.azmi@uitm.edu.my

1. Introduction

Methanol (CH3OH) is commonly used in the chemical industry as a feedstock, solvent, and fuel. The production of CH3OH is normally mass-produced from synthesis gas [1,2]. The CH3OH synthesis process has been commercialized since 1923, but the kinetics and reaction mechanism are still an opened question [3]. Syngas, also known as synthesis gas, is a fuel gas mixture mainly composed of hydrogen (H_2), carbon monoxide (CO), and carbon dioxide (CO_2). The name of syngas comes from its use as intermediates in creating synthetic natural gas and for producing ammonia or methanol [4]. At present, CH_3OH is mainly produced through the low-pressure catalytic reaction of syngas. This operating condition promotes CH_3OH formation while limiting by-product generation, with reported selectivity exceeding 99% for CH_3OH [4].

One of the main equipment in the process of CH3OH production is reactor. Heat and pressure will be applied in the reactor and the main product, which is CH3OH, is produced here. Any process upset or deviation in terms of temperature and pressure will result in the fluctuation of the production amount and thus can cause unpredictable accidents such as explosion. Heat management is important in methanol production using a tubular reactor due to the exothermic nature of the process and the reactor configuration.

One of the challenges in methanol production using a catalytic reactor is the production cost. High energy consumption and raw material prices contribute significantly to the operating and material costs. Most methanol industries have tried to maximize conversion to increase yield to overcome this problem [5]. However, maximizing conversion also leads to higher energy consumption [6]. In this case, the process objectives become interrelated because maximizing conversion and minimizing energy consumption are conflicting objectives.

Although a single objective approach can produce an optimal solution, it does not describe the tradeoff between conflicting objective functions. In addition, obtaining one solution that satisfies all objectives is often difficult. The best method to solve these problems is to implement the multi-objective optimization approach (MOO). [7] Implementing MOO to improve the optimal conditions also provides an efficient method for achieving performance reciprocity resulting from opposite actions of the operational objectives. [8].

Generating the Pareto Front (PF) is not the only MOO issue. An effective algorithm for MOO must produce a set of solutions covering the whole optimum PF while also being uniformly distributed to represent the best trade-off configuration accurately [9]. As a result, the evaluation of an MOO method commonly considers criteria such as convergence, which reflects how close the PF solutions are to the global Pareto optimal point; uniformity, which describes the even distribution of solutions along the Pareto boundary; and distribution, which represents the diversity of the solution set across the entire Pareto boundary. These requirements can be assessed using performance matrices, including hyper volume, spacing, and pure diversity [10].

Nevertheless, there is still lack of work in the published research literatures for an efficient multi-objective optimization algorithm. No algorithm can tackle all optimisation problems with the same simplicity and efficiency, according to the general theory known as the "no free lunch (NFL)" [11]. Performance on one set of problems does not guarantee similar results for other problems. The NFL theorem provides a basis for researchers to develop new strategies or improve existing methods for specific case studies. In this context, alternative MOO methods can provide benefits for industrial applications. The swarm-based meta-heuristic approaches called multi-objective dragonfly algorithm (MODA), Multi-objective Particle Swamp Optimization (MOPSO) and multi-objective Slime Mould Algorithm (MOSMA) are used to resolve optimisation problems [12].

This study primarily conducts a comparative analysis of three MOO swarm-based approaches (MODA, MOPSO and MOSMA). Therefore, this study aims to determine a suitable method for solving the multi-objective optimisation problem (MOOP) of methanol production in a fixed bed reactor. The optimisation focuses on identifying the optimum decision variables, namely reactant mole flow rate and pressure, to maximise productivity and conversion while minimising energy cost. In this study, three optimisation problems with different objective functions are investigated: (P1) maximisation of conversion with minimisation of energy cost, (P2) maximisation of conversion with minimisation of side product formation, and (P3) maximisation of productivity with minimisation of bare module cost. The multi-objective Dragonfly Algorithm (MODA), Multi-objective Particle Swarm Optimization (MOPSO), and Multi-objective Slime Mould Algorithm (MOSMA) are newly introduced for model-based optimisation of methanol production in a fixed bed reactor.

The main contribution of this study lies in the comparative application of three swarm-based multi-objective optimisation algorithms, namely MOPSO, MODA, and MOSMA, for the Aspen Plus-based optimisation of methanol production in a fixed-bed catalytic reactor. This contribution is supported by the No Free Lunch theorem, which states that no single optimisation algorithm can perform best for all optimisation problems. Therefore, different algorithms must be evaluated for specific case studies and process conditions.

Compared with previous methanol production optimisation studies, this work considers several conflicting objectives, including the maximisation of CO_2 conversion and methanol production rate, as well as the minimisation of energy cost, bare module cost, and side product formation. In addition, the optimisation methods are evaluated using Pareto Front quality indicators, namely hypervolume, pure diversity, and spacing. This allows a more systematic comparison of convergence, diversity, and solution distribution. Therefore, this study provides a more comprehensive optimisation framework for methanol production by combining process simulation, swarm-based multi-objective optimisation, and quantitative Pareto Front performance evaluation.

2. Process Modeling

The reactions for CH_3OH production that occurred during the hydrogenation of CO and CO_2 were as per followings [13]:

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H°_{298} = -90.55\ kJmol^{-1} \tag{1}$$

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2 \qquad \Delta H°_{298} = -49.43\ kJmol^{-1} \tag{2}$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \qquad \Delta H°_{298} = 41.12\ kJmol^{-1} \tag{3}$$

Based on Equations (1), (2), and (3), syngas is used in the formation of CO and CO_2, which subsequently react to produce CH_3OH through the reactions described in Equations (1) and (2). The synthesis of CH_3OH from carbon oxides commonly uses CuO or ZnO based catalysts, known as Synetix catalysts. The performance of these catalysts has been evaluated in both adiabatic and isothermal reactors. The conversion of carbon oxides to CH_3OH is an exothermic process that generally operates at high pressure and low temperature conditions, typically within 40–110 bar and 200–300 °C [14].

The production and yield of the reactor are strongly influenced by process temperature because catalytic reactions are generally exothermic. In CH_3OH synthesis, a fixed-bed reactor is commonly used due to its dynamic operating behaviour and suitability for low-pressure operation. The rate of a chemical process is generally related to its reaction kinetics. A chemical process may consist of one or several individual reaction steps [7], which are commonly referred to as elementary reactions or

elementary steps. Elementary reaction was a single reaction reactive collision between two molecules which known as bimolecular step or isomerization of a single reactant molecule which also known as unimolecular step [2].

Kinetic rate of equations that had been used in this simulation were the equations that proposed by Bussche and Forment as shown in equation (4), (5) and (6) [14]. The main reason that the equations were chosen was that the catalysts (CuO and ZnO) that were used by Bussche and Forment [14] were both have similar chemical composition and a commercial type.

$$r_{CH3OH} = \frac{k_1 P_{CO2} P_{H2} \left(1 - \frac{P_{CH3OH} P_{H2O}}{K_{eq1} P_{CO2} P_{H2}}\right)}{\left(1 + \frac{k_3 P_{H2O}}{P_{H2}} + \sqrt{k_4 P_{H2}} + k_5 P_{H2O}\right)} \quad (4)$$

$$r_{RWGS} = \frac{k_2 P_{CO2} \left(1 - K_3^{eqn} \frac{P_{H2O} P_{CO}}{P_{CO2} P_{H2}}\right)}{\left(1 + \frac{k_3 P_{H2O}}{P_{H2}} + \sqrt{k_4 P_{H2}} + k_5 P_{H2O}\right)} \quad (5)$$

The value of k obtained from the Arrhenius equation:

$$k_j = A_j \exp > B_j / RTC \quad (6)$$

Table 1
Frequency Factors for Kinetic Equation [7, 15]

Reaction Rate	Frequency Factor and Activation Energy	
k1	A	4.39517×10^{-13}
	B	36696
k3	A	345.38
	B	-
$\sqrt{k4}$	A	0.499
	B	17197
k5	A	6.62×10^{-11}
	B	124119
k2	A	1.22×10^{10}
	B	-94765
K_2^{eqn}	$10^{3066/T-10.592}$	
K_3^{eqn}	$10^{-2073/T+2029}$	

The value of A for k_1 frequency factor was estimated and determined by using parameter estimation tools Design Spec in Aspen Plus [2]. The basis of model development to produce CH_3OH was the reactor block. Based on the previous research, the reaction conditions of inlet and outlet streams between industrial data (Khark petrochemical methanol plant in Iran) and the research's data were satisfied and these data had been used as a benchmark and comparison in order to configure the Aspen Plus simulation model in this study [2]. The process configuration and operating specifications are presented in Figure 1a and Table 2. A fixed-bed catalytic reactor operating under plug flow conditions was used in this study, as shown in Figure 1b.

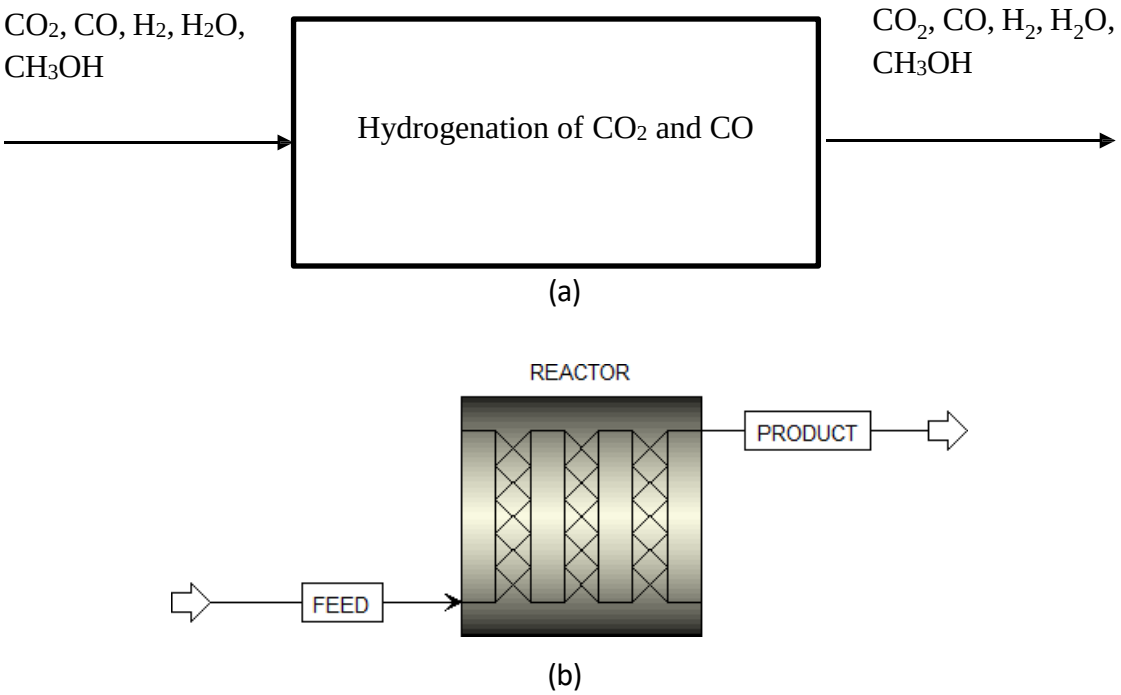


Fig. 1. Basis for model development of methanol in the fixed bed reactor

Table 2
Industrial data [2]

Parameter	Value
Temperature	225 ºC
Pressure	82 bar
Feed CH_3OH molar flowrate	142.2 kmol/hr
Feed CO molar flowrate	2256.24 kmol/hr
Feed CO_2 molar flowrate	1398.3 kmol/hr
Feed H_2O molar flowrate	28.44 kmol/hr
Feed H_2 molar flowrate	37920 kmol/hr
Length of reactor	10 m
Number of pipes	5947
Void fraction of bed	0.285

Based on the literature review, the reaction was considered as a polarity condition and under the pseudo reaction type [1]. The method of reaction that was opted in the Aspen Plus was Langmuir-Hinshelwood-Hougen-Watson (LHHW) due to the non-linear equation [15]. The equations and data for the driving force expression, kinetic reaction and adsorption expression were presented in equation (4) – (6) and Table 1.

3. Multi-objective optimisation (MOO) method

In the MOO approach, the optimum solution is represented by a trade-off set of feasible alternatives that may not be optimal for every objective function. A multi-objective optimisation problem (MOO), consisting of m objective functions, n variables, p inequality constraints, and q equality constraints, can be expressed as shown in Equation (7).

$$Min\ f(x_i) = [f_1(x_i), f_2(x_i), \ldots, f_m(x_i)] \quad (7)$$

Subject to

$u_j(x_i) \geq 0$, *j*= 1, 2, …, *p*

$v_k(x_i) \geq 0$, *k*= 1, 2, …, *q*

$x_i^{(L)} \leq x_i \leq x_i^{(U)}$, i= 1, 2, …, *n*

The population-based optimisation is well suited to solving such a problem and generating an equilibrium solution set [12].

3.1. Multi-objective dragonfly algorithm (MODA)

The MODA depends on static and dynamic swarming skills, including separation, alignment, cohesiveness, attraction to food supply (i.e., towards optimality), and deterrence from enemies (i.e., non-movement towards non-optimality) [16]. Figure 2 shows the MODA flow diagram.

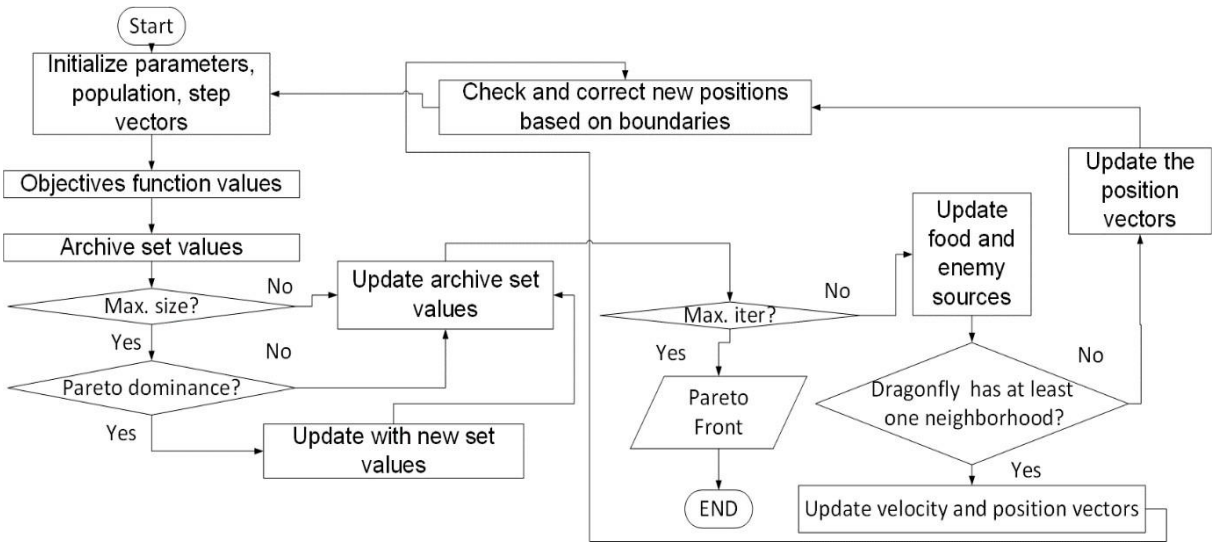


Fig. 2. Basic procedure of MODA

The Dragonfly Algorithm (DA) is a stochastic, population-based, and nature-inspired optimisation method. It is developed based on the swarming behaviour of dragonflies, particularly the exploration and exploitation mechanisms. In DA, static swarming behaviour represents exploration, where small groups of dragonflies move in different directions while searching for food. In contrast, dynamic swarming behaviour represents exploitation, where larger groups move in a common direction during migration or prey hunting [12]. These two behaviours form the basis of the optimisation process in the DA method. The algebraic equations describing the DA components are presented in [12].

3.2 Multi-objective Slime Mould Algorithm (MOSMA)

The Slime Mould Algorithm [17] (SMA) is a population-based stochastic inspired by the oscillation behaviours of slime mould in nature. The method applies a positive–negative feedback mechanism to identify suitable food paths and is based on three main behaviours: grabble, wrap, and approach. The grabble behaviour represents collision avoidance among slime moulds during food searching.

The wrap behaviour describes velocity matching between slime moulds, while the approach behaviour represents movement towards the food source. The mathematical representation of the SMA algorithm involving the three fundamental principles of grabble, wrap, and approach phenomena is given in detail from [17]. The flowchart of MOSMA is depicted in Figure 3.

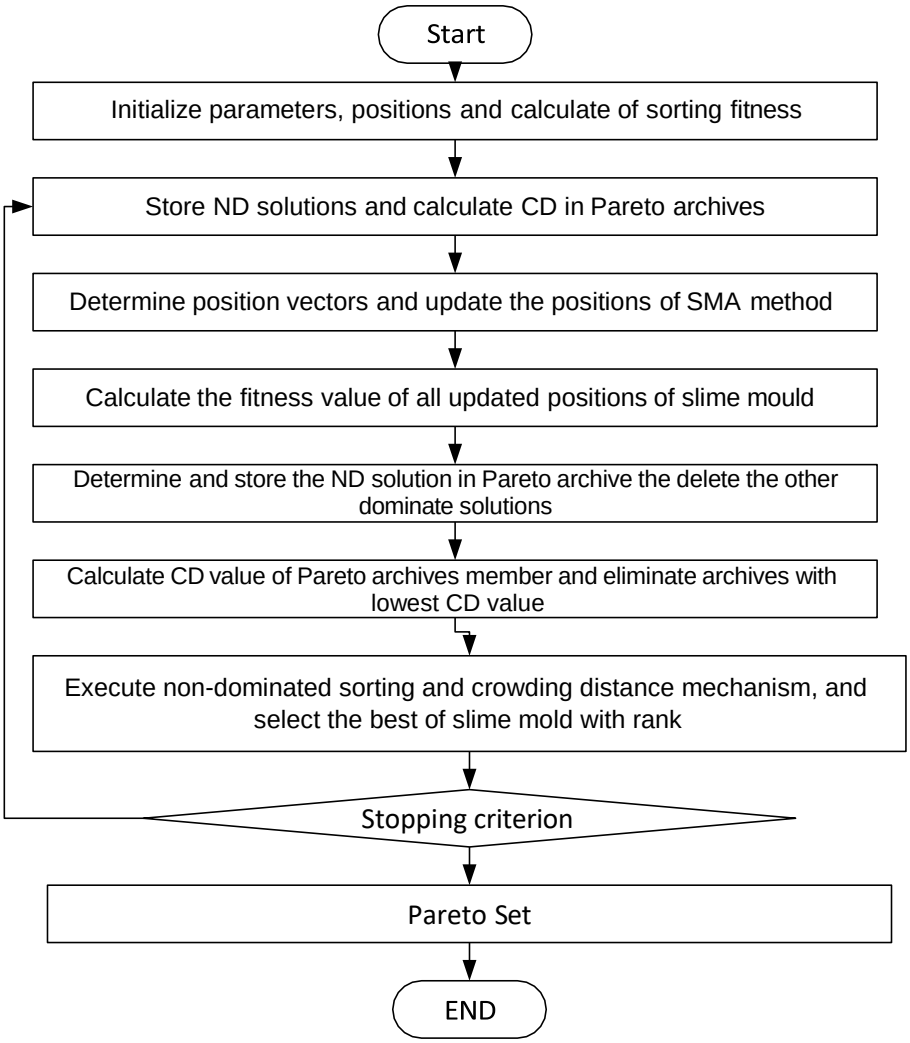


Fig. 3. The flowchart of MOSMA

3.2 Multi-objective Particle Swamp Optimization

MOPSO employs the concept of Pareto dominance in PSO and is capable of dealing with multi-objective optimisation problems. PSO is a heuristic algorithm that simulates the behaviour of a group of organisms moving in the search-space based on the best local and global positions found at any given time [16]. A population in PSO is made up of a specific number of particles. Each particle is characterised by its velocity and position. MOPSO consists of two main components: the archive controller and the grid system. The archive controller manages the addition and removal of solutions in the archive. During each iteration, the non-dominated solutions from the current population are compared with the existing solutions in the repository. When a new solution lies outside the current grid boundary, the grid system is adjusted to include the new solution space [12]. Figure 4 depicts the MOPSO flowchart.

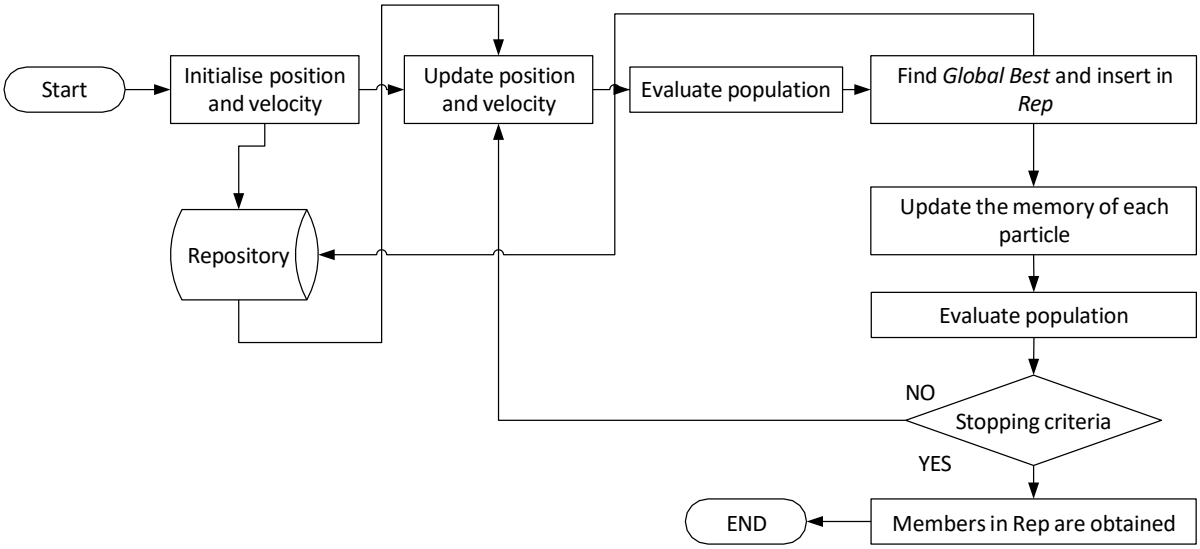


Fig. 4. Basic schematic of MOPSO

3.4 Problem Optimisation Formulation

Here, three MOO problems included are:

- simultaneous min/max of conversion (X_{CO2}) with energy cost (P1)
- min/max conversion (X_{CO2}) with energy cost (P2)
- min/max of product F_{CH3OH} with bare module cost (CBM) (P3)

The constraint involved in these MOO problems is the maximum allowable product temperature. The optimised variables are F_{H2} and pressure in the reactor [7]. The objective function is the min-function type (to minimise) [18]. The max function, symbolised as min ($-X_{CO2}$), maximises yield X_{CO2}. Equations 10 to 13 express Problems (P) 1-3.

The five optimisation objectives were selected to represent the main technical and economic considerations in methanol production. CO_2 conversion and methanol production rate were included to evaluate reactor performance and process productivity. Energy cost was considered because methanol synthesis is strongly affected by operating pressure and heat management, which directly influence process utility requirements. Bare module cost was included to represent the capital cost associated with reactor design and sizing. In addition, side product formation was considered because the formation of water affects product quality, separation requirements, and overall process efficiency.

These objectives are strongly interrelated and may conflict with one another. For example, increasing reactor pressure may improve CO_2 conversion and methanol production, but it may also increase energy demand and equipment cost. Similarly, operating conditions that favour higher conversion may also influence the formation of side products. Therefore, the simultaneous consideration of conversion, product rate, side product formation, energy cost, and bare module cost provides a more comprehensive optimisation framework. This allows the optimisation procedure to identify practical trade-off solutions rather than focusing only on maximum production or minimum cost.

Problem 1:

$$\min_{u(t),p(t_0)} \ (-X_{C02})$$

$$\min_{u(t),p(t_0)} \; cost_E$$

$$3.6 \times 10^4 \frac{\text{kmol}}{\text{hr}} \leq F_{\text{H2}} \leq 3.8 \times 10^4 \text{ kmol/hr}$$

$$1\text{MPa} \leq \text{P} \leq 8.5\text{MPa}$$

$$X_{C02} = \frac{\text{inlet molar flowrate } CO_2 - \text{outlet molar flowrate } CO_2}{\text{inlet molar flowrate } CO_2} \quad (10)$$

$$cost_E = cost_{\text{Q}} + cost_{compress} \quad (11)$$

$$cost_{\text{Q}} = 1.242 * |\text{g}| \quad (12)$$

$$cost_{compress} = \frac{ParmFsrream}{17.1} \text{hi} \frac{P}{P_{arm}} \text{j}^{0.286} - 1\text{k} \quad (13)$$

The X_{C02} is conversion of CO_2, F_{H2} is the mole flow rate of H_2, and F_{stream} refer to the mole flow rate of inlet mixture (reactant).

Problem 2:

$$\min_{u(t),p(t_0)} \; (-X_{C02})$$

$$\min_{u(t),p(t_0)} \; F_{\text{H20}}$$

$$3.6 \times 10^4 \frac{\text{kmol}}{\text{hr}} \leq F_{\text{H2}} \leq 3.8 \times 10^4 \text{ kmol/hr}$$

$$1\text{MPa} \leq \text{P} \leq 8.5\text{MPa}$$

$F_{\text{H20}}$is mole flow rate of H_2O (side product).

Problem 3:

$$\min_{u(t),p(t_0)} \; (-F_{C\text{H30H}})$$

$$\min_{u(t),p(t_0)} \; CBM$$

$$3.6 \times 10^4 \frac{\text{kmol}}{\text{hr}} \leq F_{\text{H2}} \leq 3.8 \times 10^4 \text{ kmol/hr}$$

$$1\text{MPa} \leq \text{P} \leq 8.5\text{MPa}$$

$F_{C\text{H30H}}$is mole flow rate of CH_3OH (main product). Where CBM is bare module cost which can be represented as Equation 14, where *l* and *d* refer to length and diameter reactor.

$$CBM = 1780(l^{0.87})(d^{1.23})(2.86 + 1.694 \times FM \times (10.01 - 7.408\ln(P) + 1.395 \times \ln(P^2))) \times P \quad (14)$$

The equation 13 and 14 are derived from Peters et al. [19] which are standard economic function in designing plug flow reactor.

3.5 Integration of MATLAB Code with Aspen Plus

The MOO framework was developed by integrating MATLAB with Aspen Plus through ActiveX Automation. The MODA, MOSMA, and MOPSO solvers were implemented in MATLAB, while the program script was written in an m-file to enable direct interaction with the Aspen Plus model.

Figure 5 illustrates the integration between the Aspen Plus simulation model and the MOO framework in MATLAB. First, MATLAB sends a command to open Aspen Plus. Next, the required input data are transferred from MATLAB to Aspen Plus for process simulation. MATLAB then executes the optimisation procedure using the selected MOO approach.In this case, 'Apwn Document' is the programmatic identifier of an OLE-compliant COM server, and ActiveX is the server's default interface [20].

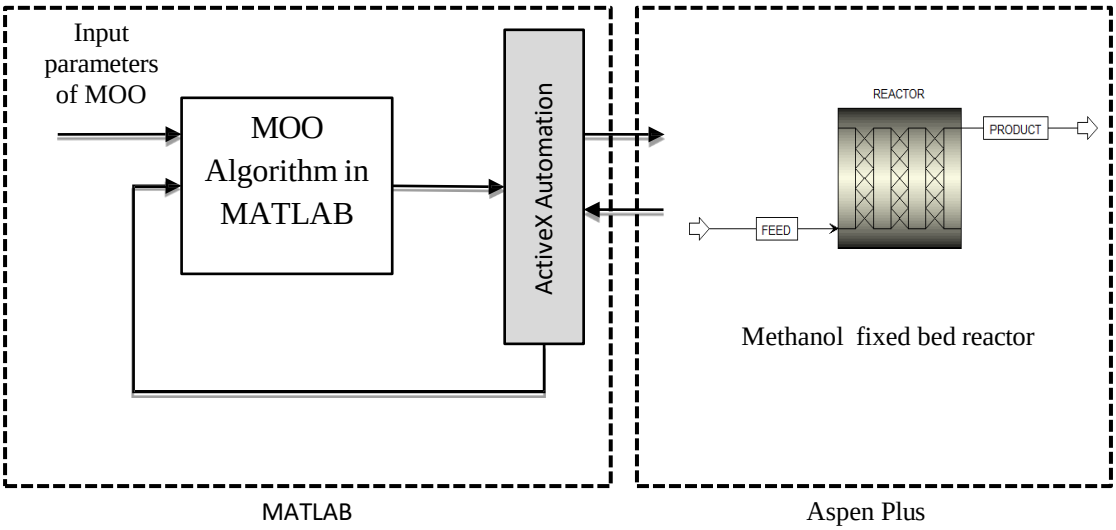


Fig. 5. MOO Algorithm scheme with Aspen Plus

3.6 MOO performance metrics (Quality indicators)

The performance of the MOO techniques was evaluated through statistical analysis of the non-dominated (ND) points obtained from the Pareto optimal (PO) solutions. The assessment was based on three performance metrics: spacing (S), hypervolume (HV), and pure diversity (PD). Spacing (S) is used to describe the distribution of ND points along the Pareto Front (PF). The HV metric measures the total rectangular area covered by the PF vectors within the objective space. Meanwhile, PD is used to evaluate the diversity and uniformity of the PO solutions. The description and mathematical formulation of those metrics can be found in [21-22].

Although this study compares MOPSO, MODA, and MOSMA using Pareto Front quality indicators, computational efficiency was not evaluated in detail. The optimisation framework was linked with Aspen Plus through MATLAB, and the total runtime may be influenced by both the optimisation algorithm and the Aspen Plus simulation execution time. Therefore, future work should include CPU time, convergence speed, and number of function evaluations to provide a more complete comparison of the computational performance of the algorithms. This is particularly important for large-scale or real-time optimisation applications in industrial methanol production.

4. Results and discussion

4.1 The simulation and validation results from the ASPEN Plus simulator

In the catalytic reactor model, CH_3OH synthesis had been taken place and would produce CH_3OH as the main product along with other components like H_2, CO, CO_2 and H_2O. The results of the outlet stream S2 molar flowrate for all of the components by simulation using Aspen Plus are shown in Table 3.

Table 3
Comparison Data for Product Stream

Component	Industrial Data (kmol/hr)	Aspen Plus simulation data (kmol/hr)	% Error (Aspen Plus simulation)
CH_3OH	2775	2762.45	0.45
H_2	31870	31894.90	0.08
CO	399	420.61	5.42
CO_2	620	613.68	1.02
H_2O	813	813.06	0.01

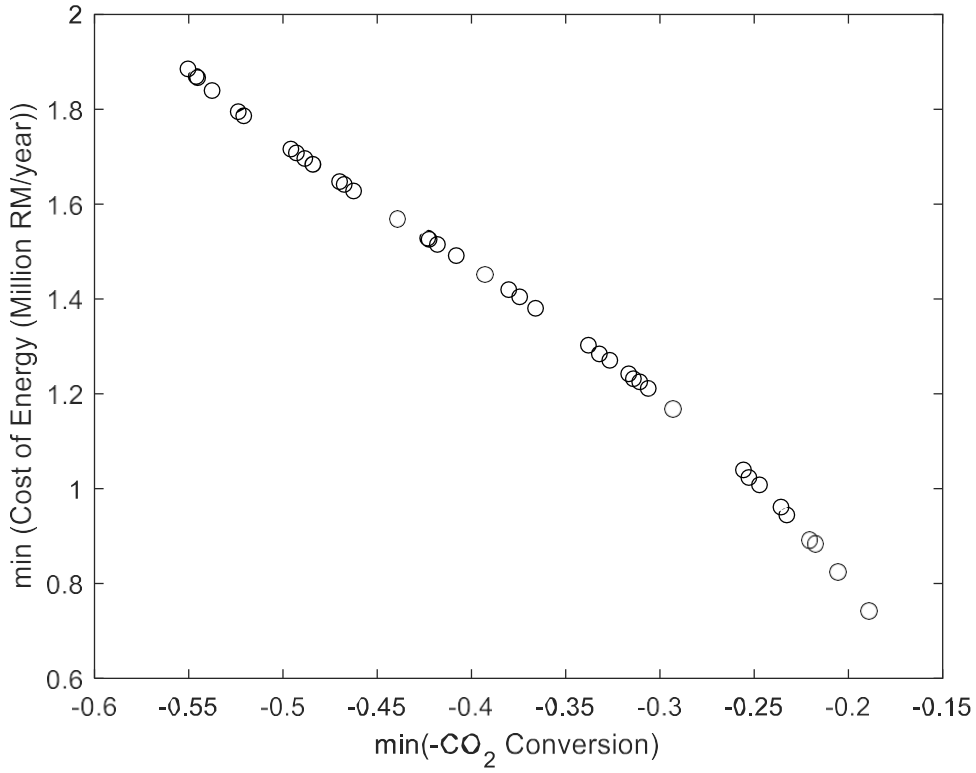
In order to validate the model, the results from simulation were compared with the industrial data. Table 3 shows that the Aspen Plus simulation produced a CH_3OH product molar flowrate with an error of 0.45% compared to the industrial data. The maximum percentage error for all simulated parameters was below 5.5%. These results indicate that the Aspen Plus model provides reasonable agreement with the industrial data and can be used to evaluate the effect of changes in process parameters.

4.2 MOOs results

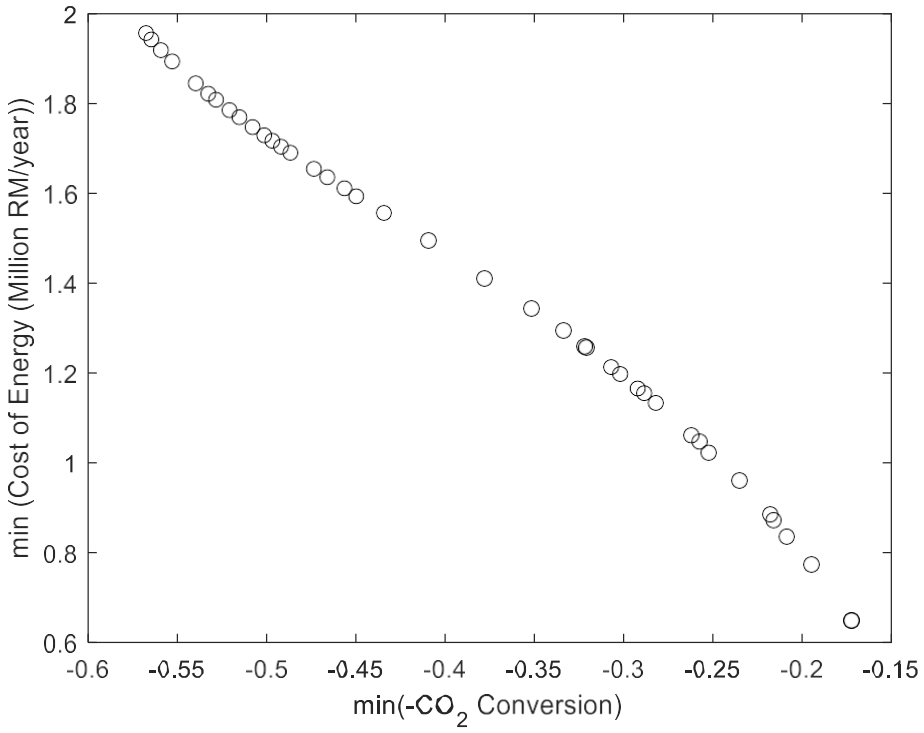
Figures 6, 7, and 8 present the PFs obtained using the MODA, MOSMA, and MOPSO methods for optimisation problems P1, P2, and P3, respectively, while Table 4 summarises the values of S, HV, and PD. Based on visual observation, the PFs generated by MOPSO and MOSMA showed a more suitable distribution of non-dominated (ND) points. In addition, the Pareto optimal solutions were distributed more evenly across the PF.

Table 4
Results performance metrics of MOPSO, MODA, MOSMA

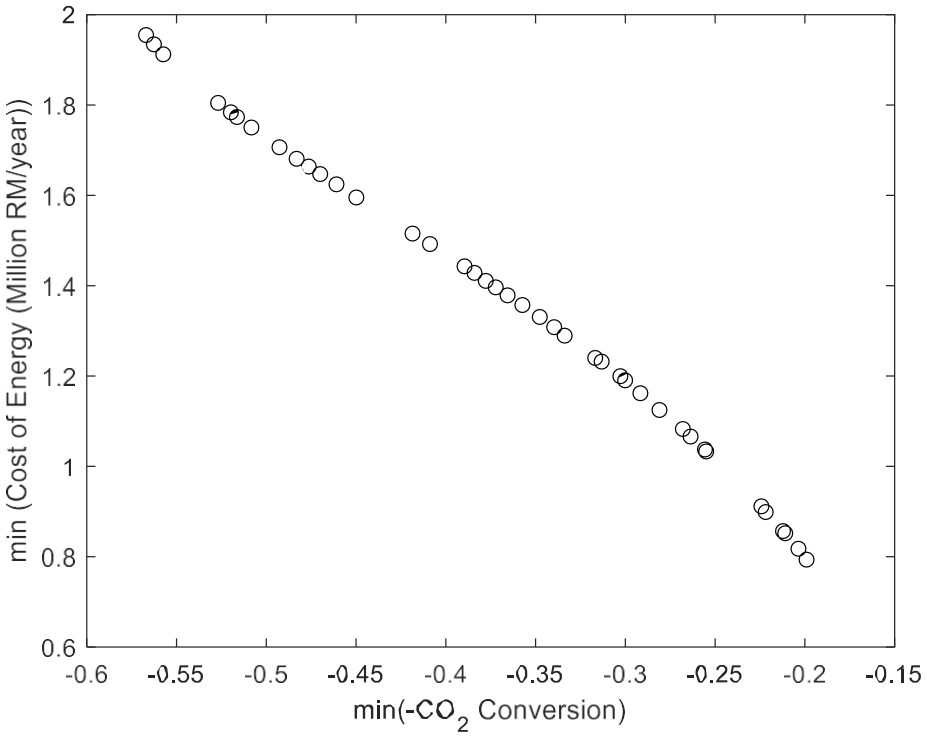
	MOPSO			MODA			MOSMA		
	P1	P2	P3	P1	P2	P3	P1	P2	P3
PD ($x10^3$)	1.021	40.637	138.72	0.816	44.185	135.13	1.309	50.071	143.22
S	0.010	3.391	21.368	0.019	5.238	23.486	0.023	4.390	31.452
HV	0.220	103.64	4707.6	0.219	101.89	4694.3	0.221	102.38	4725.8



(a) MODA

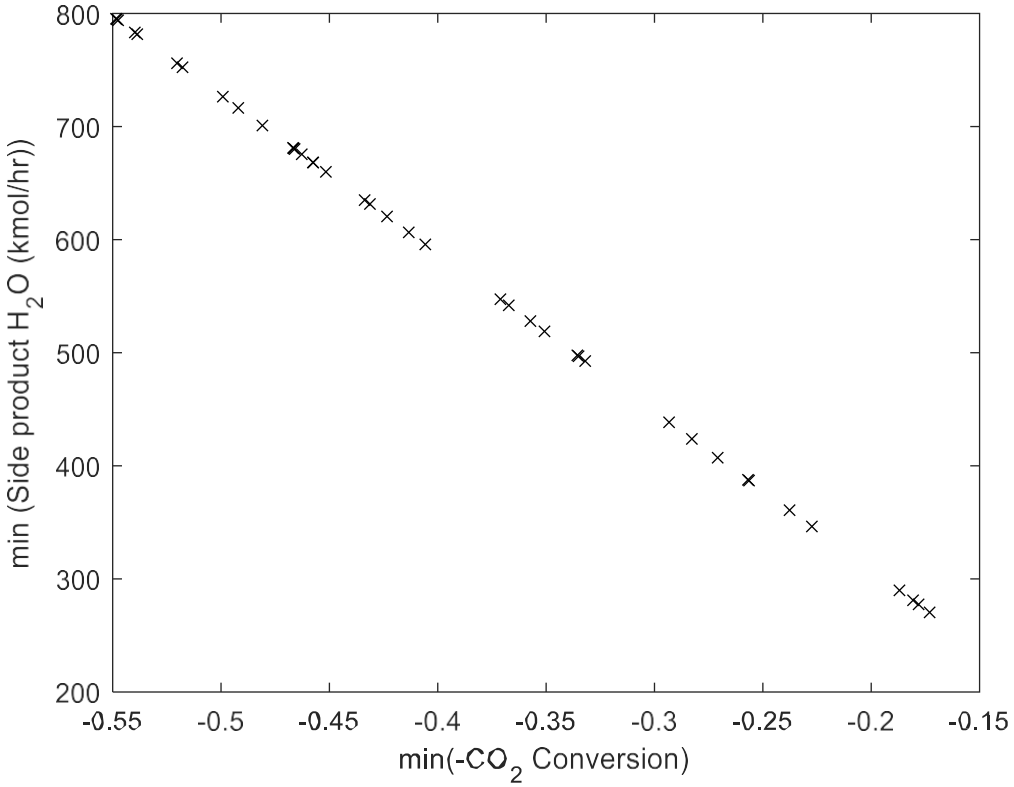


(b) MOSMA

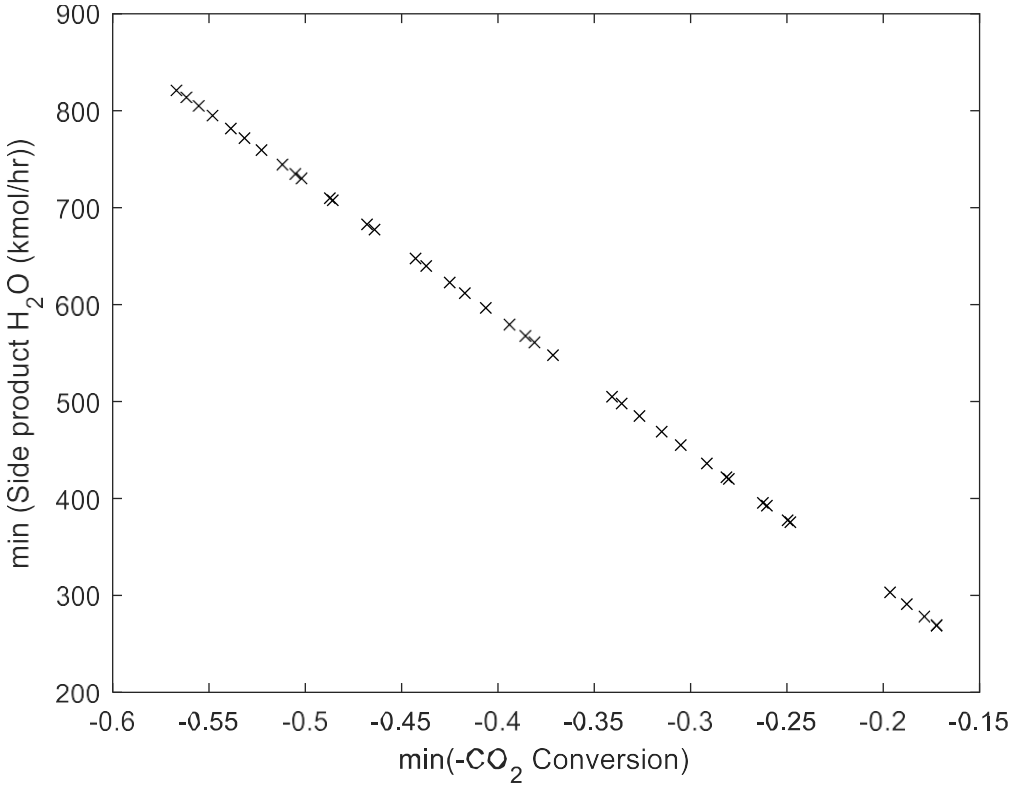


(c) MOPSO

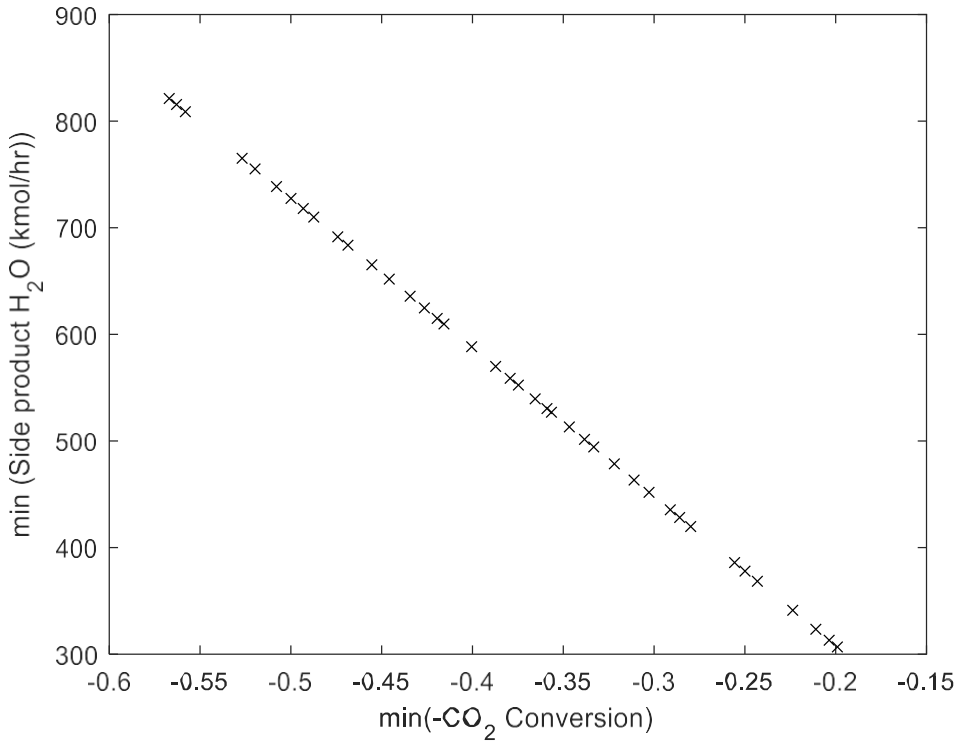
Fig. 6. (a)MODA, (b) MOSMA, (c) MOPSO Pareto fronts for Problem 1



(a) MODA

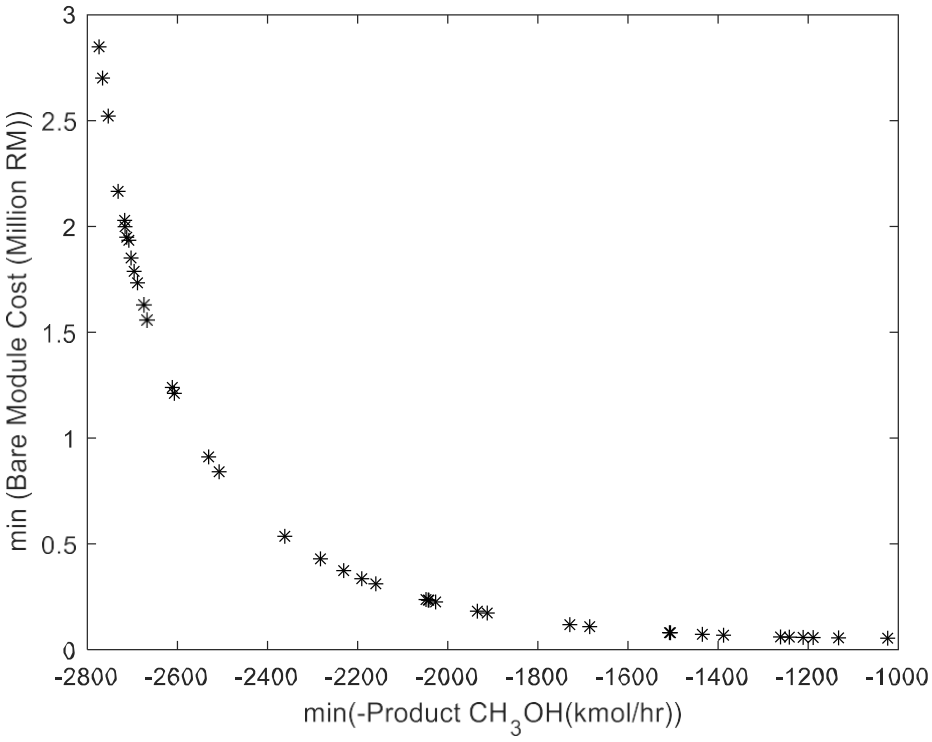


(b) MOSMA

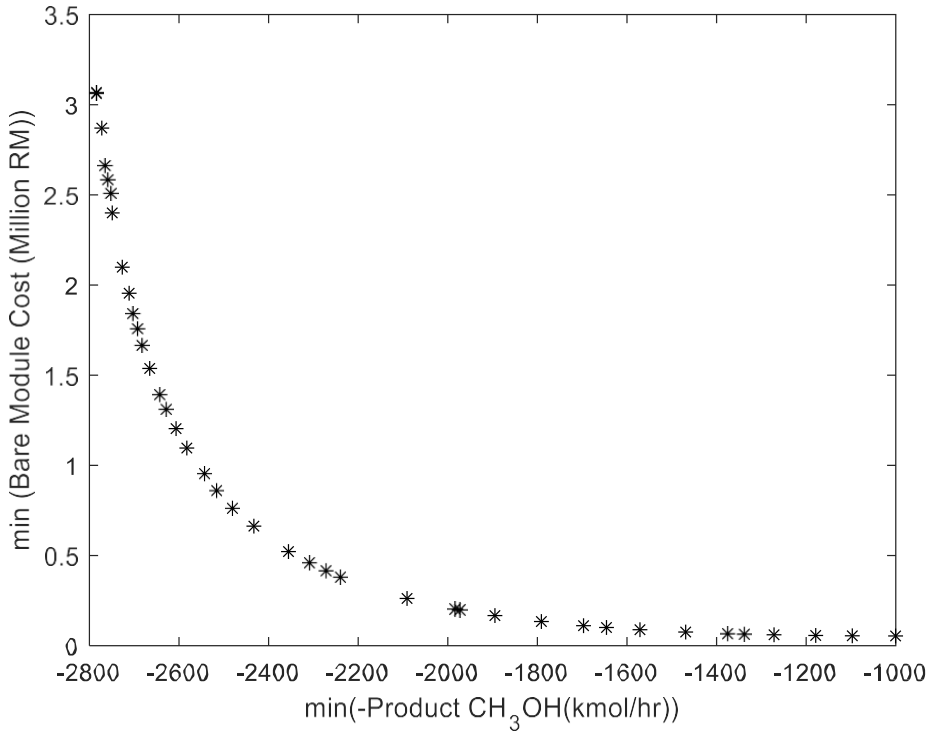


(c) MOPSO

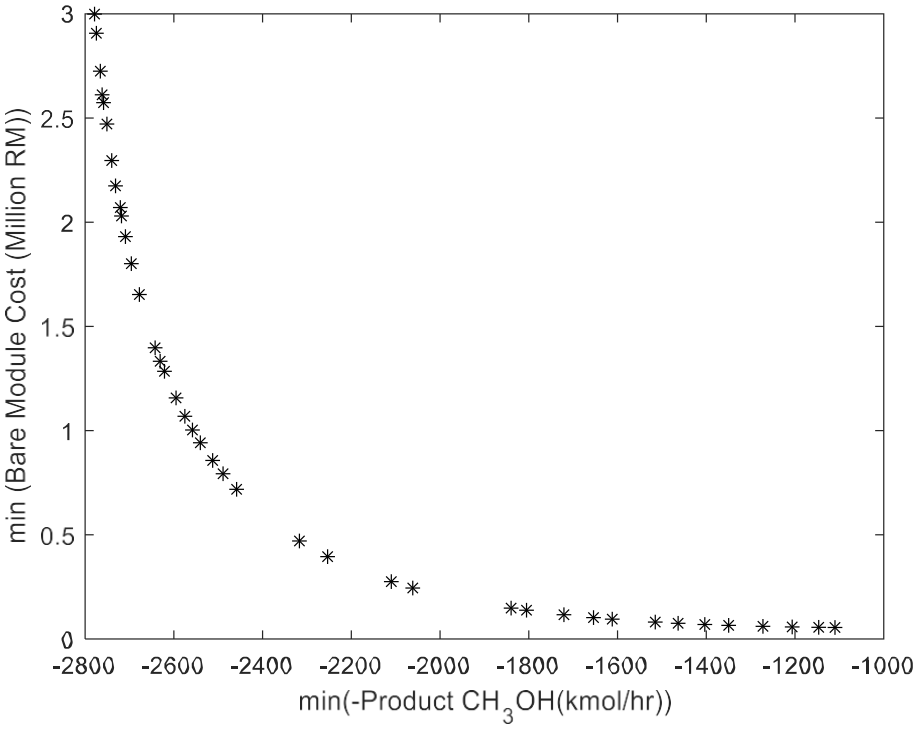
Fig. 7. (a)MODA, (b) MOSMA, (c) MOPSO Pareto fronts for Problem 2



(a) MODA



(b) MOSMA



(c)

Fig. 8. (a)MODA, (b) MOSMA, (c) MOPSO Pareto fronts for Problem 3

MODA showed a less uniform PF for both problems because the non-dominated points were concentrated in specific regions rather than being evenly distributed. Finding solutions segregated in a part of the optimal PF outperforms other potential non-dominated points and thus does not include a workable approach to the MOO problem [23].

Table 5 presents the high, low, and intermediate points for the three MOO problems, representing the PF ranges formed by the non-dominated (ND) points. Finding solutions that are concentrated in a section of the optimal PF outperforms other potential ND points, hence it is not possible to find a practical solution to the MOO problem in this way [24].

Table 5 shows that MOSMA achieved a highest conversion of 0.567, a highest product rate of 2784.147 kmol/hr, the lowest energy cost of 0.773 Mil. RM/year, and a CBM of 0.054 Mil. RM, while MODA produced the lowest side product formation at 270.399 kmol/hr. For the intermediate points obtained using MOSMA, the conversion, product rate, energy cost, CBM, and side product values were 0.409, 2515.53 kmol/hr, 1.494 Mil. RM/year, 0.859 Mil. RM, and 278.277 kmol/hr, respectively.

However, these results alone are insufficient to evaluate the coverage and quality of the non-dominated (ND) points because they depend on the extreme objective values and the variation of the ND solution sets. Therefore, further evaluation using performance metrics is required for PF selection. The effectiveness of the PF in terms of distribution, convergence, and diversity was assessed using the S, HV, and PD metrics. The spacing metric (S) was used to evaluate the distribution of consecutive ND points along the PF. As shown in Table 4, MOPSO produced the smallest S value for both problems, indicating a more uniform PF distribution. This is because the S metric is based on the standard deviation of the minimum Euclidean distances between ND points, where smaller distances indicate that the points are located closer to one another. In fact, as S $\approx$0, all ND points of MOPSO are homogeneous spaces [25].

Furthermore, the PD metric is employed to investigate the multiplicity of un-reiterated solutions with a more significant disparity of ND points along the PF, resulting in higher PD. From Table 4,

MOSMA produced the highest PD values for both problems, indicating greater diversity in the solution sets obtained along the Pareto Front. On the other hand, MODA solutions for P1,P2 and P3 need more diversity, for example, the smallest PD value, because some of the ND points are aggregated in separated zones [26].

The HV values presented in Table 4 reflect both the convergence and distribution of the Pareto Front. This metric is calculated based on the total volume formed by hypercubes between a selected reference point W (such as the worst objective function values in the objective space) and each non-dominated (ND) point on the PF. The HV indicator evaluates an approximation's proximity to PF [27] In other words, the closer the solution reaches reference point W, the closer it gets to convergence. Therefore, the HV metric is used to evaluate both the distribution of the non-dominated (ND) solutions and their convergence toward the optimal Pareto Front (PF). As a result, MOSMA achieved the highest HV value, indicating better convergence and diversity of the solution set. A higher hypervolume generally reflects a closer approximation to the Pareto Front [28]. Based on the selected Pareto Front quality indicators, MOSMA showed relatively better performance in terms of solution diversity and hypervolume for the methanol production optimisation problems considered in this study.

Figure 9 presents the relationship between the decision variables (FH_2 and pressure) and the objective functions, namely conversion, energy cost, CBM, side product formation, and product rate, based on the Pareto Front obtained from MOSMA. The decision variable plots indicate that pressure has a significant influence on conversion, product rate, CBM, and energy cost. Other decision variable, i.e. F_{H2} is almost constant, with some amount of scatter.

Changes in pressure affect reaction equilibrium by shifting the system toward a state with either fewer or greater moles of gas [29]. According to Le Chatelier's principle, an increase in pressure (or decrease in volume) shifts the equilibrium toward the side with fewer gas moles, while a decrease in pressure (or increase in volume) favours the side with more gas moles. Since the reactant side contains a greater number of gas moles than the product side, increasing the reactor pressure shifts the equilibrium toward CH_3OH formation, resulting in higher methanol production. A similar trend was observed for CO_2 conversion, which increased with increasing reactor pressure.

The optimisation results have practical engineering significance for industrial methanol production. The increase in CO_2 conversion and methanol production rate indicates improved feed utilisation and reactor productivity. At the same time, the reduction in energy cost and bare module cost reflects the economic benefit of selecting more efficient operating conditions. The inclusion of side product formation is also important because lower side product generation can reduce downstream separation requirements and improve overall process efficiency. Therefore, the obtained Pareto solutions provide useful trade-off information for selecting operating conditions that balance production performance, energy consumption, equipment cost, and product quality.

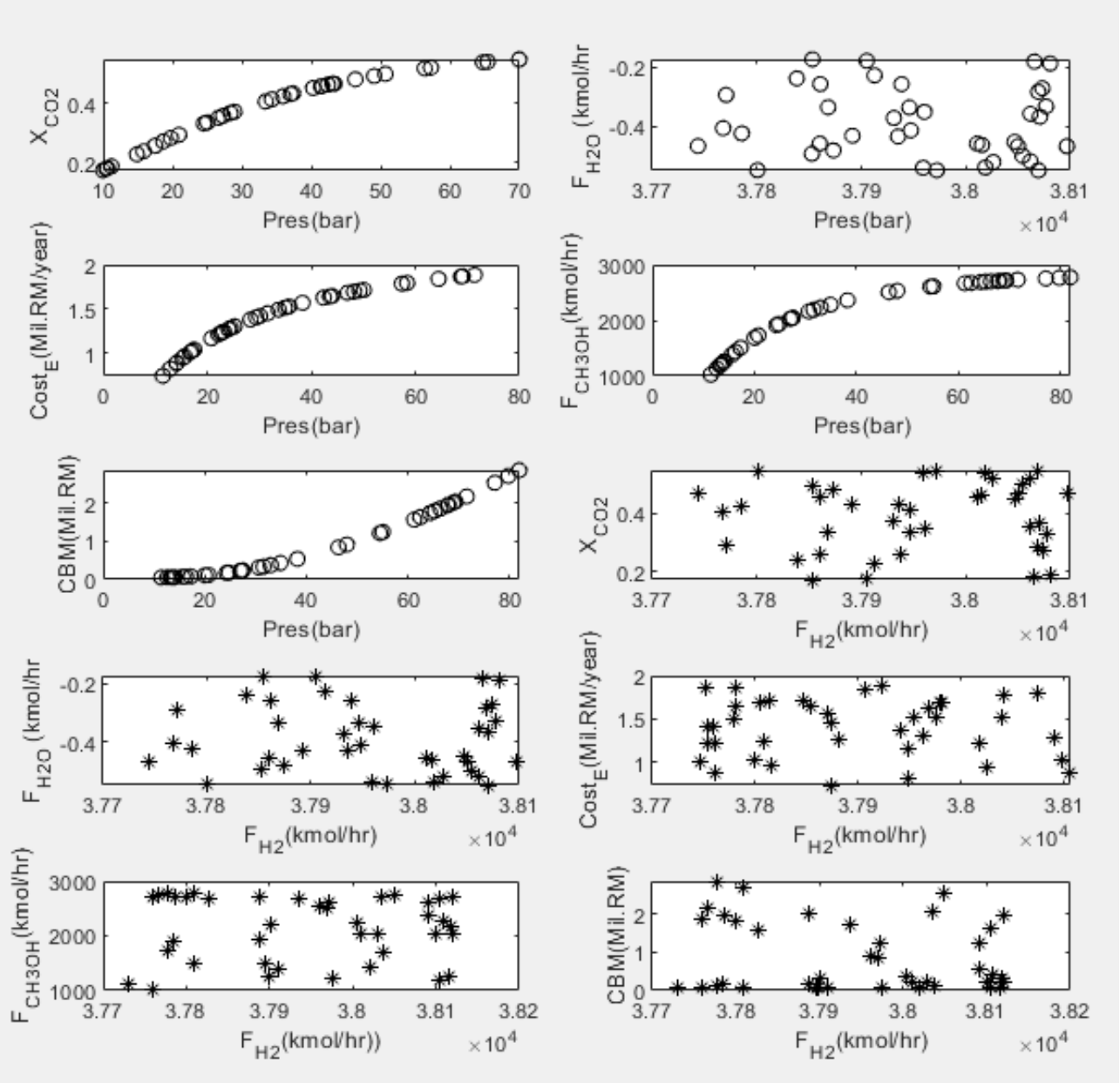


Fig. 9. Conversion, energy cost, CBM, side product and product rate relation with decision variables (FH_2 and pressure)

5. Conclusion

The MODA, MOSMA, and MOPSO methods were applied to optimise CH_3OH production in a fixed-bed catalytic reactor under a reactor temperature constraint. The optimisation aimed to maximise conversion and product rate while minimising side product formation, bare module cost (CBM), and energy cost. The performance of these methods was compared based on the Pareto Fronts obtained for the constrained MOO problems.

Based on the comparative evaluation using performance indicators such as spacing, pure diversity, and hypervolume, MOSMA showed better performance in terms of Pareto Front convergence and solution diversity. The extreme values obtained were a conversion of 0.567, a product rate of 2784.147 kmol/hr, an energy cost of 0.773 Mil. RM/year, a CBM of 0.054 Mil. RM, and a side product formation of 270.399 kmol/hr. Among the decision variables considered, pressure showed the strongest influence on the optimisation results.

The optimisation results also indicate potential environmental and carbon-utilisation benefits. Higher CO_2 conversion suggests that more CO_2 can be converted into methanol, which supports the use of CO_2 as a carbon feedstock for value-added chemical production. In addition, lower energy cost and reduced side product formation may improve the overall process efficiency and sustainability of methanol production. Nevertheless, the actual environmental benefit depends on factors such as the CO_2 source, hydrogen production route, and overall energy supply. Therefore, future work should include life-cycle assessment and carbon footprint analysis to quantify the environmental impact of the proposed optimisation framework.

This study has several limitations. The optimisation results depend on the accuracy of the Aspen Plus simulation model and the assumptions used in developing the fixed-bed catalytic reactor. Although the model was validated against industrial data and showed acceptable agreement, several practical effects were not fully considered, including catalyst deactivation, detailed heat-transfer limitations, pressure drop variation, equipment fouling, and plant-wide operational disturbances. In addition, the optimisation was conducted using a steady-state simulation framework. Therefore, the obtained Pareto solutions should be interpreted as simulation-based optimisation results.

Future work should focus on experimental or plant-scale validation of the obtained Pareto solutions to confirm their practical applicability. In addition, dynamic optimisation should be considered to evaluate the performance of the proposed framework under changing feed composition, temperature, pressure, and production demand. Catalyst deactivation should also be incorporated into the reactor model because catalyst activity may decrease over long-term operation and affect conversion, product rate, and operating cost. Furthermore, uncertainty assessment should be conducted to examine the effect of uncertain kinetic parameters, feed conditions, and economic data on the optimisation results. These future studies will improve the robustness and industrial relevance of the proposed optimisation framework for methanol production.

Conflict of interest

The authors declare that there are no conflicts of interest related to the publication of this manuscript. The authors received no financial support, funding, grants, or any other form of compensation that could have influenced the study outcomes. This research was conducted without any commercial or financial relationships that could be perceived as a potential conflict of interest.

Data availability

The datasets generated and/or analysed during the current study are available from the corresponding author upon reasonable request.

Declaration of Generative AI and AI-assisted technologies in the manuscript preparation process

During the preparation of this manuscript, the authors used ChatGPT to improve language clarity, refine sentence structure, and enhance overall readability. All generated content was carefully reviewed, revised, and validated by the authors, who assume full responsibility for the accuracy and integrity of the final published work.

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Table 5
Extreme points in PF for the MOO problems

MOO Problem (objectives)	Low extreme point			Intermediate point			High extreme point		
	MOPSO	MODA	MOSMA	MOPSO	MODA	MOSMA	MOPSO	MODA	MOSMA
Problem 1:									
Max X_{CO2},	0.199	0.205	0.195	0.409	0.393	0.409	0.566	0.550	0.567
Min $cost_E$ (Mil.RM/y)	0.793	0.824	0.773	1.492	1.452	1.494	1.955	1.8851	1.956
Problem 2:									
max X_{CO2},	0.199	0.170	0.179	0.401	0.405	0.406	0.567	0.548	0.566
min F_{H2O}(kmol.hr^{-1})	306.797	270.399	278.277	588.392	595.797	596.578	821.235	795.346	820.751
Problem 3:									
max F_{CH3OH} (kmol.hr^{-1})	1109.876	1023.549	1000.380	2512.553	2507.44	2515.531	2778.734	2773.95	2784.147
Min CBM (Mil.RM)	0.055	0.0541	0.054	0.857	0.841	0.859	2.998	2.848	3.063