Journal of Petroleum Science and Technology 13(2): 38, 2023, Pages 46-66
DOI:10.22078/jpst.2023.5021.1853

Journal of Petroleum Science and Technology
Research Paper
https://jpst.ripi.ir/

Optimization of an Integrated Natural Gas to Polypropylene Plant Using Sinus-Cosine Algorithm

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Abstract
The main aim of this study is to simulate and optimize an integrated industrial natural gas (NG) to polypropylene (PP) plant (NGTPP). The optimization in this study aimed to increase the PP productivity as an objective function of the optimization problem. This plant consisted of four subunits: NG to synthesis gas, synthesis gas to methanol, MTP , and PTPP units. After sensitivity analysis of all possible effective parameters, reformer temperature($T_{Ref.gas}$), methanol reactor temperature(T_{MeOH}), methanol reactor pressure (P_{MeOH}), hydrocarbon return flow ratio to methanol reactor (R_{HC}), PP reactor temperature(T_{PPR}), PP reactor pressure(P_{PPR}), Ticl4(M_{Ticl4}) and TEA(M_{TEA}) inlet flow to PP reactor have been selected. These parameters were optimized using the Sinus-Cosine Algorithm(SCA). Optimal obtained results showed that the $T_{Ref.gas}$, T_{MeOH}, P_{MeOH}, R_{HC}, T_{PPR}, P_{PPR}, M_{Ticl4}, and M_{TEA} equal 875.53 0C, 225.91 0C, 140.87 bar, 0.7, 55.19 0C, -1.96 bar, 107.97 kg/h, and 3.93 kg/h, consequently. Maximum PP productivity was 7058.85 kg/hr at the optimum point.

Keywords: Large Scale Optimization, Single Objective Optimization, Aspen HYSYS and Plus, SCA, Polypropylene Production.

Introduction
Reducing oil resources and limiting access to these resources as a strategic material used for energy supply and production of various materials has created many incentives to find new ways to reach energy and produce different materials previously produced with oil [1]. One of these strategic materials is propylene, widely used today in gas conversion and petrochemical industries. Propylene is widely used as a restorative material for producing plastics and polymers such as PP and polyacrylic acid. Due to the widespread use of this substance, the demand for propylene is expanding daily, so new methods for producing this material are essential. Global demand for propylene is rising (Fig. 1). This trend of global demand for polypropylene was reported by Nexant company.

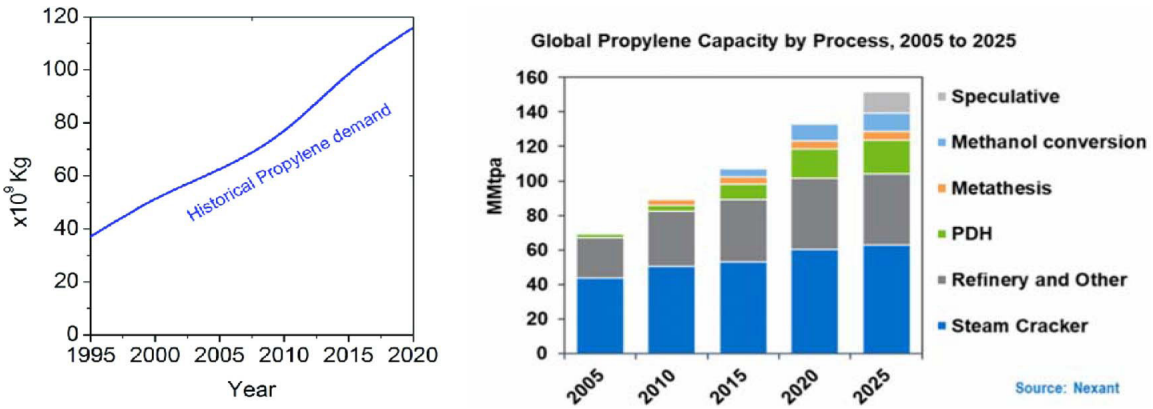

Fig.1. The Global propylene production capacity.

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Received 2023-01-30, Received in revised form 2023-08-27, Accepted 2023-08-20, Available online 2024-02-12

Most propylene is currently produced via steam cracking of naphtha, but targeted processes based on selective propane dehydrogenation (PDH) or using methanol as an intermediate are also being investigated.

The coal-to-propylene route has been of particular interest in China.

As mentioned above, propylene production has been reduced using steam cracker technology.

It has led to the developing of "in-case" propylene production facilities, particularly PDH and methanol-to-propylene (MTP) plants. Since the methods of methanol production are diverse, one of the methods considered for producing methanol is using natural gas as a feedstock for methanol production, which eliminates the dependence on crude oil for producing propylene [2]. Currently, propylene is sold in the world markets for about 820 dollars per ton, and the price of methanol as a raw feed is about 360 dollars per ton. Therefore, converting methanol to propylene will not be of much benefit. On the other hand, considering the price of natural gas, which is about 12 cents per cubic meter, the MTP method fed with natural gas is very economical, and the cost of producing propylene is compared to the method whose feed is petroleum derivatives.

Fig. 2 shows the costs of propylene production with different methods. According to the figure, it is clear that the production of propylene with the MTP method is low compared to other methods, and the sale price of propylene in Southeast Asia is 1,241 $/ton, which is a very suitable market for selling this product.

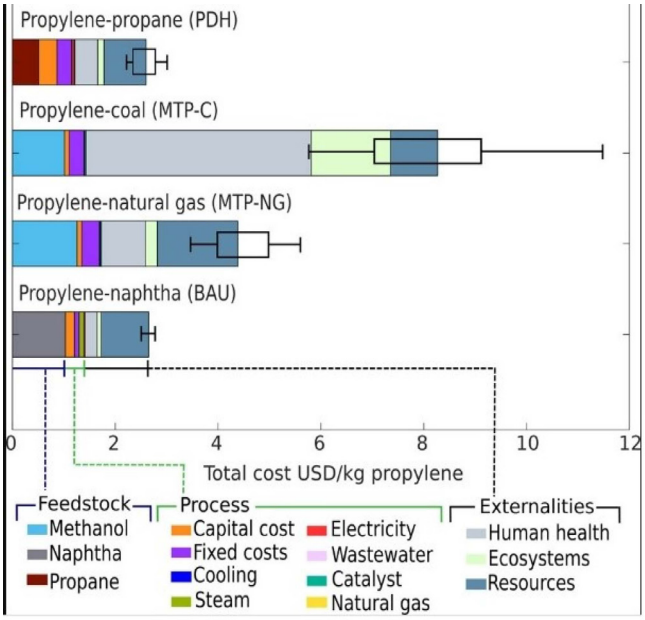

Fig. 2 Cost of propylene production with different methods [3].

Currently, there is no specific method for producing propylene in the Middle East region, and propylene is mainly produced by cracking, which is about 85%, or is produced as a byproduct of other processes. It is absent in the Middle East region, and propylene is mainly produced through cracking, which is about 85%, or as a byproduct of other processes. The rest of the propylene required is imported from other countries. Nevertheless, the Middle East region is considered a strategic region for expanding the MTP method due to its vast gas resources. Among polyolefin, polypropylene (PP) is one of the most demanded plastics in the world market [4]. PPs are widely used in the daily life of today's people due to advantages such as low production cost, reduced environmental effects [5], good processability [6], lightness, high melting temperature, and having desired mechanical properties including strength [4,7]. Moreover, impact resistance and transparency are widely used in the plastic industry [7, 8] PPs from packaging materials [9]. They are used in producing toys, pipes, glue, fiber, film, household appliances, and special electronics, aircraft, and automobile applications [4, 10, 11].

In addition, PPs, as a clean material, are also prominent in the discussion of environmental equipment. This title is not only due to the absence of halogen compounds and benzene in the structure of PP but also due to their recyclability [7].

PP is one of the most widely used materials in the health and medical sector due to its transparency, lack of pollution, lightness, and cheapness [12]. PP was produced for the first time in 1594 AD in Milan, Italy [13]. The most common type of catalysts for PP production are Ziegler-Natta catalysts [14] ($MgCl_2$/$TiCl_4$/Lewis base based on $MgCl_2$ [15]). More than 90% of PP catalysts are produced with Ziegler-Natta catalyst [16, 17]. Catalysts used in the industry for PP production include catalysts (4th generation Ziegler-Natta with external electron donors), dimethoxysilane, and fifth generation with internal electron donors. They are diatomaceous [5]. PP is one of the most widely used polymers, whose global production reached 35.8 million tons in 2003. The annual growth of global demand for PP between 2003 and 2019 has reached about 16.7%. The highest demand in the industries of fiber-reinforced devices production, filament yarn production, plastic injection, and pneumatic injection [18]. The characteristics of PP compared to other polymers are [18]:

- Reasonable price of propylene as feed for PP production compared to other feeds,
- The reasonable price of PP compared to other polymers,
- The specific weight of PP is light,
- Increasing the use of this material due to the increase in the quality of this material with new methods,
- Use of this substance in the medical industry,
- Using PP as an alloy with other polymers.

The technology of converting natural gas into propylene is a process that takes place in several stages and generally consists of three or five parts (if the feed has impurities such as hydrogen sulfide), an amine purification unit, and a sulfur recycling unit as additional steps. It is formed [19, 20]:

- Gas sweetening process (in case of impurity).
- Synthesis gas production unit.
- Conversion of synthesis gas to methanol.
- Conversion of methanol to propylene\

Materials and Methods

Subunits Description of NG to PP

Synthesis Gas Production Unit

Synthesis gas (syngas) is a mixture of hydrogen gas and carbon monoxide in different proportions, and it is used to produce various substances such as methanol, ethanol, dimethyl ether, etc. Due to the many applications of syngas and the use of this material for the synthesis of ammonia,

gasoline, methanol, dimethyl ether, etc., it is of interest to industries [21]. According to CHIYODA corporation data, Fig. 3 shows the schematic of synthesis gas production with various feedstock and various products that used syngas as feedstock. Synthesis gas production from natural gas has various methods, including partial oxidation, steam reforming, autothermal, dry reforming, and tri-reforming, discussed below [22, 23]. In the method of steam reforming, metal is mainly used as a catalytic material, and the reactions that occur in this process include two reactions: the reforming reaction of methane with steam and the water-gas shift reaction:

$H_4+H_2O \leftrightarrow CO+3H_2$ $H_{298}=2.1\times10^5$ kJ/kgmole (1)

$CO+H_2O \leftrightarrow CO_2+H_2$ $H_{298}=-4.2\times10^4$ kJ/kgmole (2)

Reaction 1, the main reformer reaction (steam methane reforming (SMR)), is endothermic, and the other one, a water gas shift reaction (WGS), is exothermic. Still, the total enthalpies show that the process is endothermic, and a lot of energy must be consumed to carry out the process [24]. In partial oxidation of methane gas, the process feed is mixed with oxygen at the top of the reactor. It reacts with combustion in the burner part and produces synthetic gas at a temperature of 1250 degrees Celsius with a ratio of (H_2/CO= 2). The gases that come out of the top of the reactor in this process include CO, H_2, and CO_2, and this reaction is exothermic. The autothermal reforming method consists of partial oxidation and steam reforming. It eliminates the problem of coke generation [24].

Considering that the main cause of global warming is CO_2 and CH_4 gas, using the dry reforming of methane gas to produce synthesis gas according to reaction 3 can effectively prevent global warming [25]. In the dry methane reforming method, nickel and cobalt catalysts are used. In this process, the hydrogen-to-carbon monoxide ratio is around 1.0 [26]. The dry reforming reaction is:

$CH_4+CO_2 \leftrightarrow 2CO+2H_2$ $\Delta H_{298}=+247.3$ kJ/mol (3)

Carbon deposition and deactivating the catalyst of this process is one of the biggest problems of the dry reforming process [27]. The tri-reforming method consists of three methods: steam reforming, dry reforming, and partial oxidation of methane gas. In this process, the ratio of hydrogen gas produced to carbon dioxide gas is between 1.0 and 2.0, which is suitable for producing various types of liquid hydrocarbons and Fischer-Tropsch synthesis. In this process, the problem of coke formation on the catalyst of the dry reforming process is solved, and it increases the lifespan of the catalyst [28]. In the methanol unit, for the synthesis of methanol, the ratio of hydrogen to carbon monoxide is significant, and this ratio in the range of 3.5 to 5 is suitable for the synthesis of methanol, so a method must be chosen to provide this ratio [29]. The main feed of the MTP conversion process is synthesis gas, which can be supplied using steam methane reforming and partial oxidation. Of course, the unwanted side product of carbon dioxide is also produced in these two methods, which must try to reduce the amount of this product. There are different methods to minimize the byproduct of carbon dioxide. One of these methods is to return carbon dioxide gas to the incoming feed to prevent the equilibrium reaction's progress and increase the percentage of feed conversion to carbon monoxide, but there are problems with this method. One of them is reducing the ratio of hydrogen to carbon monoxide, which increases the production of carbon monoxide. The other is the catalyst of the steam reforming method, which is made of nickel metal based on alumina, and this catalyst cannot do this. Still, the researchers for two methods of Tri-reforming and dry reforming have developed new catalysts that solve this problem for producing synthesis gas, which has not yet been industrialized. A schematic of the synthesis gas production unit is shown in Fig. 4 [30].

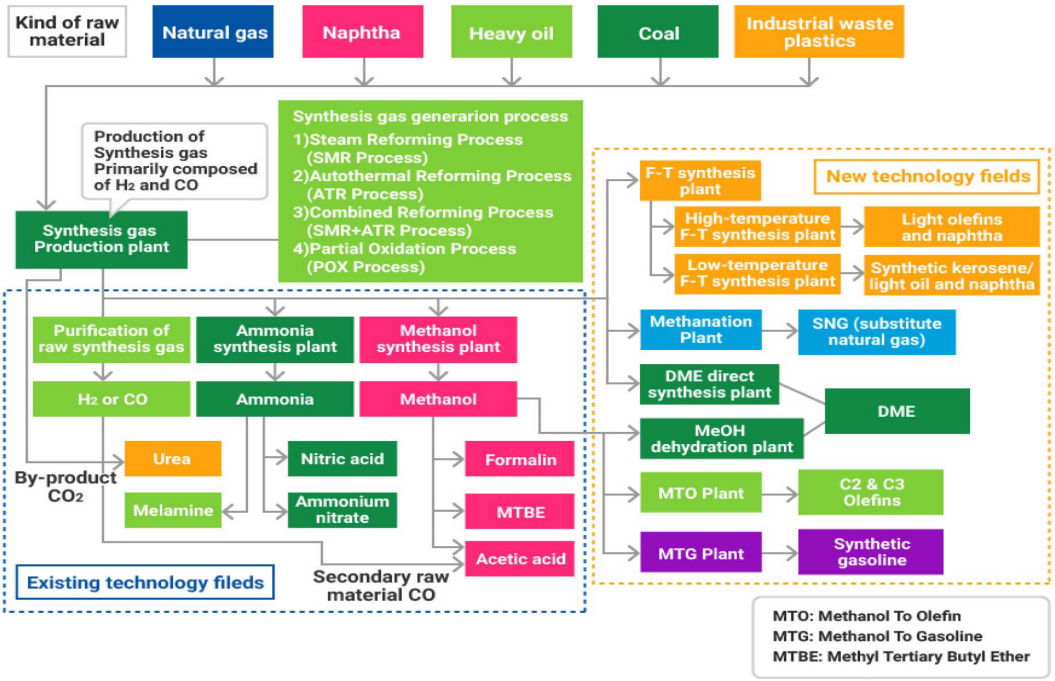

Fig. 3 The synthesis gas production routes and derivatives.

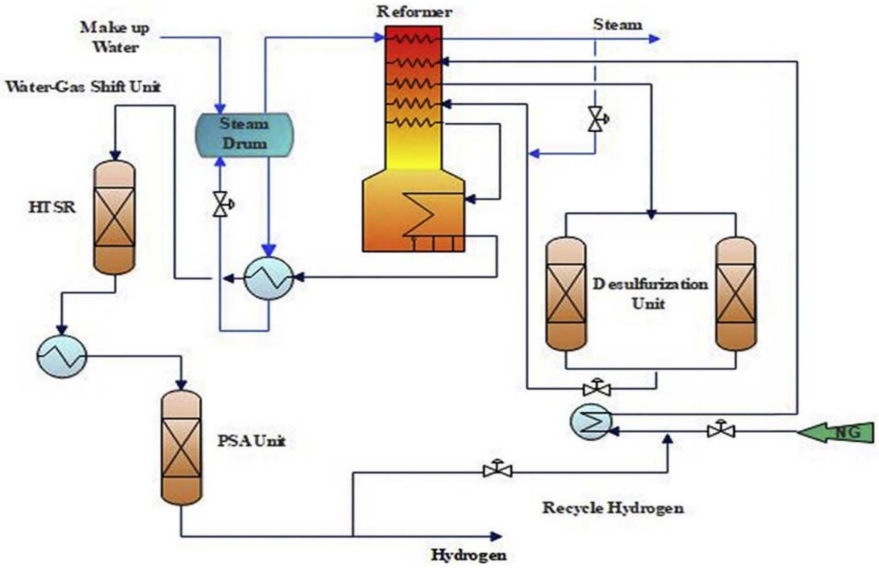

Fig. 4 Schematic of the synthesis gas production unit [31].

Synthesis Gas to Methanol Process

According to Fig. 5, methanol synthesis consists of three sections for increasing the pressure of synthesis gas using compressors, a reactor, return flows, and a section for separating and purifying products. Synthesis gas is converted into methanol by performing a general exothermic reaction under operating conditions of 50 to 100 bar pressure and 210 to 270 °C using a copper alumina catalyst [32]. Synthesis gas is converted to methanol using the following reactions [33]:

$CO + 2H_2 \leftrightarrow CH_3OH + Q$ (5)

$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O + Q$ (6)

Methanol to Propylene Process

Because of the reduction of oil resources, it seems very attractive to obtain new methods for producing propylene; one of these methods is converting methanol to olefin (MTO). In the MTO process, ethylene is the main product, and propylene is produced as a side product. Lurgi first proposed the MTP method by optimizing the propylene production process as a byproduct of the MTO process. The efficiency of propylene production in reactions has increased greatly, and the reactions of this process are carried out in a fixed-bed reactor with a ZSM-5 zeolite catalyst.

To specialize in the process of producing propylene from methanol, Lurgi company started to conduct tests with a pilot plan, and for this process, they chose the ZSM-5 zeolite catalyst that they had tested before and started to optimize and check the reaction conditions and the result that was obtained is as follows. It turned out that the propylene production reactor with a fixed bed is the best for this process and has the highest efficiency for propylene production. However, in this process, ethylene and gasoline with high octane number are also produced in a small amount as side products. The MTP process was implemented in Norway in 2002. Propylene with high efficiency and suitable quality was produced to be converted into polymer derivatives. Also, appropriate operating conditions such as temperature, pressure, material residence time, etc were obtained for this process, and the catalyst used for this process was shown to have a long life.

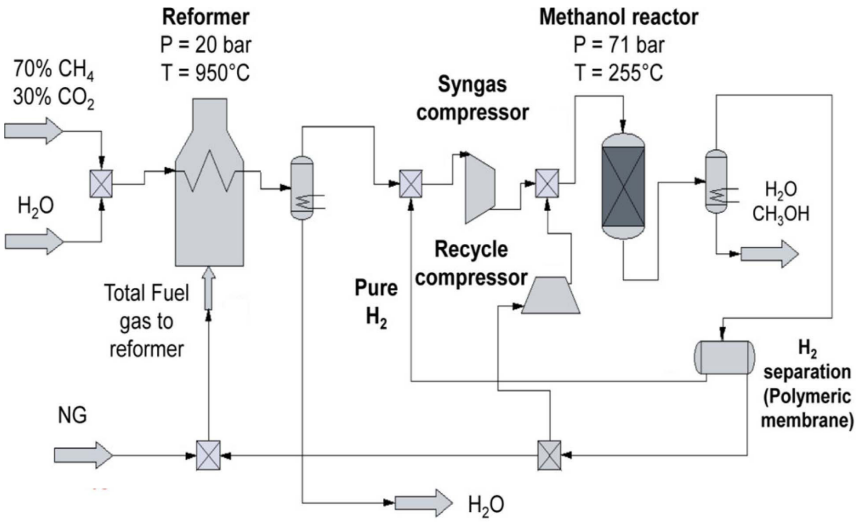

Fig. 5 Schematic of the methanol production from natural gas [34].

The MTP process is a new method that eliminates dependence on crude oil and is very cost-effective and economical for countries that use natural gas resources. Also, this process is due to the use of synthetic gas feed consisting of hydrogen and carbon dioxide in the environmental discussion, which has been successful and, to some extent, reduces the pollution caused by the propylene production process [33]. Considering the new capacities of propylene and its derivatives, which are expected to create significant changes in the world's propylene market shortly, various studies have been conducted on different methods of propylene production, economic estimation, simulation, and optimization of this process. However, due to the newness of the method of converting MTP, only a few researchers have investigated the equipment, simulation, and optimization of this process using hybrid Aspen and MATLAB software and have studied and tested more in the catalyst modification of this process. According to the studies conducted in optimizing petroleum and petrochemical processes, optimization by SCA has been used in limited studies.

Propylene to Polypropylene (PTPP) Process

The growth of polypropylene production capacity is predicted to be 5.7% from 2015 to 2025 AD, while demand growth is predicted to be 7%. With this growth rate, polypropylene will be one of the most demanded thermoplastic resins in the world. This growth is due to the extensive properties of polypropylene, its abundance, and the relatively low costs of polypropylene production. The first generation of Ziegler-Natha catalysts was invented in 1950. Finally, in 1980, the fourth generation of Ziegler-Natha catalysts was invented. Recently, Montel company has invented the fifth generation of Dieter-based Ziegler-Natta catalysts, which can produce one hundred kilograms of polymer per gram of catalyst and has increased the melt flow index (MFI) to 1,700. Single-site catalysts such as metallocene have been introduced as the next generation of consumable catalysts in polypropylene production, creating properties that were not imagined before. Polypropylene with variable properties ranging from mono-arrangement to co-arrangement can be produced by modifying the catalyst composition.

In contrast, the consumption of metallocene and other single-site catalysts is lower than expected. The polypropylene production process has two bulk slurry ring (tubular) reactors, and one gas phase reactor uses a floating bed as a series. The design is based on the product with 80% homo-polymer and 20% rubber phase. Random homo-polymer or copolymer is also produced in loop reactors. Because the concentration of propylene in bulk polymerization is higher than in gas-phase polymerization, a higher catalytic activity ((polymer pond)/(catalyst pond)) is observed. A pump with an axial flow creates the rotation of materials (circulation) in the reactor ring. The circulating cold water inside the second wall of the reactor controls the temperature. The reactor slurry phase usually has 50% by weight concentration. The polymerization of polymer and its solubility leads to the limitation of the closing mass inside the reactor, the reactor's temperature, and the copolymer's composition. Hydrogen content is limited by its solubility. High hydrogen solubility leads to cavitation (vacuum creation) in the pump. The slurry phase of the reactor is discharged from the second annular (tubular) reactor into the flash distillation device. The substantial stream of uncombined monomers is sent to the propylene recovery column and returned to the reactor with fresh propylene. The polymer is sent to the floating bed reactor, where the rubber phase is produced. This process uses the advanced catalyst of the fourth-generation Ziegler-Natta, which is called the fifth-generation Ziegler-Nata catalyst [35].

Simulation and Optimization of NG to Poly Propylene Process

In any process, increasing productivity and reducing energy consumption and environmental pollution are of great importance, and process optimization is for this purpose [36]. Optimization means obtaining the best solution for the parameters and variables in the system so that the system can reach the objective function defined for it. The objective function can contain one or more parameters.

The simulation of NG to propylene and propylene polypropylene conversion unit and its single-objective optimization is discussed in this section. Aspen HYSYS v11 and Aspen PLUS v11 software were used for simulation, and optimization code was written in MATLAB software environment.

Thermodynamic Models Used in Simulation

Aspen One package has comprehensive and robust thermodynamic and physical methods to minimize errors. Therefore, this package increases calculation accuracy regarding hydrocarbon and non-carbon compounds. PRSV is the property package used in this process. Choosing different property packages in some units is necessary to obtain high-accuracy results. In Table 1, all the property packages used in other units have been tabulated.

Table 1 Property packages used in all methanol to polypropylene.

Unit	Property package
Syngas unit	PRSV
Methanol unit	Peng Robinson
MTP unit	Peng Robinson + UNIQUAC

Process Description and Simulation of NG to Syngas Process and Simulation

NG consists of simple hydrocarbons such as methane (CH_4) and heavier hydrocarbons such as ethane (C_2H_6), propane (C_3H_8), and butane (C_4H_{10}). In some gas fields, ethane gas has a significant portion (10% or more), while heavier gases have a much smaller portion among gas compounds. N_2, CO_2, and H_2S compounds are associated with NG, and their share in existing gas reservoirs differs. Among the unfavorable factors in gas compounds, water causes problems in transmission lines and lowers the calorific value of gas. Therefore, water and disturbing compounds are removed in the dehumidification unit of gas refineries. Finally, after applying the reforms, the transmission lines deliver the output gas to the target consumer groups.

Among the available feeds for NG, according to Table 2, the Kangan feed was selected for the simulation of the synthesis gas production unit. Feed specifications and operating conditions are given in Table 3.

Table 2 Types of NG feed and molar percentage of its ingredients.

		Gas field name				
Formula	Component Name	Tehran	Sarkhoon	Khangiran	Bidboland	Kangan
CH_4	Methane	87.7	88.089	98.548	84.157	88.02
C_2H_6	Ethane	4.70	3.42	0.647	9.5	4.13
C_3H_8	Propane	1.74	1.27	0.069	3.744	1.29
C_4H_{10}	Iso-Butane	0.37	0.29	0.018	0.413	0.28
C_4H_{10}	n-Butane	0.42	0.37	0.039	0.768	0.38
C_5H_{12}	i-Pentane	0.13	0.12	0.018	0.125	0.16
C_5H_{12}	n-Pentane	0.10	0.07	0.021	0.101	0.10
C_6H_{14}	Hexane	0.08	0.09	0.14	0.016	0.19
N_2	Nitrogen	4.70	5.75	0.50	0.715	5.45
CO_2	Carbon dioxide	0.05	0.53	0.00	0.412	0.00

Table 3 Specifications of input feed to synthesis gas unit.

Parameter	Value
Mass flow (kg/h)	35370
Temperature(°C)	65
Pressure (bar)	15
Mole fraction	
CH_4	0.8802
C_2H_6	0.0413
C_3H_8	0.129
n-C_4H_{10}	0.0038
i-C_4H_{10}	0.0028
n-C_5H_{12}	0.001
i-C_5H_{12}	0.0016
n-C_6H_{14}	0.0019
N_2	0.0
CO_2	0.0545

According to Fig. 5, NG is sent to the syngas production unit and divided into two parts:
1) gas entering the reformer under the name of fuel (S-3)
2) gas input to the reformer under the name of feed (S-4)
The proportion of gas input as fuel (S-3) compared to feed (S-4) is determined based on the heat load required for the reformer to produce synthesis gas (800-900 °C). In the current simulation, the ratio of fuel flow intensity to total NG is considered 0.35-0.45. The SMR process to produce syngas from NG is implemented in a sample of industrial reformers. Two equilibrium reforming reactors (EVR-100 and Reformer) and conversion reactor (R101-PreReformera), as well as conversion reactor (F-101), have been used as the primary reformer to simulate the SMR process in the Aspen HYSYS environment. The primary reformer (F-101), which has the role of a burner and fuel, operates under a pressure of 15 bar, and its gas output has a temperature of 1203 °C. The output stream (S-6) from the heat exchanger E-107, mixed with the stream (S-7), enters the prereformer reactor. Water, methane, carbon monoxide, and hydrogen are among the compounds that are at the output of (S-10), and to adjust the rate of conversion of hydrogen to carbon monoxide as well as methane reforming, the existing flow is directed to the equilibrium reactor (R101-prereformer) and the water and unreacted carbon monoxide is converted into hydrogen and carbon dioxide in the reactor (EVR-100). The ratio of hydrogen to carbon monoxide in converting natural gas to propylene from the MTP route equals 1.62. According to the mentioned materials, the kinetics of the SMR process can be divided into the following two categories:
1) Transformation type reactions
2) Equilibrium type reactions
Table 4 shows all conversion reactions where the hydrocarbons present in the feed are sorted from C1 to C10. Due to the reaction of hydrocarbons heavier than C1 in the reformer (F-101), the feed stream of the steam reformer (S-12) lacks hydrocarbons heavier than methane. The reactions of the equilibrium type that the water-gas displacement reaction and SMR take place in this secondary reforming are presented In Table 5.

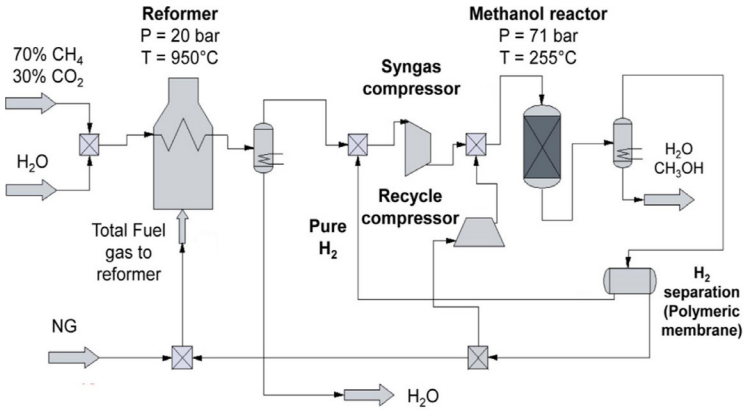

Fig. 5 Schematic of the methanol production from natural gas [34].

Table 4 List of primary reformer conversion reactions.

Reaction stoichiometric formula	Eq. No.	Conversion (%)
$CO + 0.5O_2 \rightarrow CO_2$	(1)	100
$H_2+0.5O_2 \rightarrow H_2O$	(2)	100
$CH_4 + 2O_2 \rightarrow CO_2+2\ H_2O$	(3)	100
$4C_2H_6 + 7O_2 \rightarrow 4CO_2+6\ H_2O$	(4)	100
$C3H_8 + 5O_2 \rightarrow 3CO_2+4\ H_2O$	(5)	100
$2\ i\text{-}C_4H_{10} + 13O_2 \rightarrow 8CO_2+10\ H_2O$	(6)	100
$2\ n\text{-}C_4H_{10} + 13O_2 \rightarrow 8CO_2+10\ H_2O$	(7)	100
$2\ i\text{-}C_5H_{12} + 13O_2 \rightarrow 8CO_2+10\ H_2O$	(8)	100
$2\ n\text{-}C_5H_{12} + 13O_2 \rightarrow 8CO_2+10\ H_2O$	(9)	100

Table 5 List of types of primary reformer equilibrium reactions.

Reaction stoichiometric formula	Eq. No.	Equilibrium reactions of primary pre-reforming
$C_2H_6 + 2H_2O \rightarrow 2CO + 5H_2$	(10)	Steam ethane reforming
$C_3H_8 + 3H_2O \rightarrow 3CO + 7H_2$	(11)	Steam propane reforming
$i\text{-}C_4H_{10} + 4H_2O \rightarrow 4CO + 9H_2$	(12)	Steam i-butane reforming
$n\text{-}C_4H_{10} + 4H_2O \rightarrow 4CO + 9H_2$	(13)	Steam n-butane reforming
$i\text{-}C_5H1_2 + 5H_2O5 \rightarrow CO + 11H_2$	(14)	Steam i-pentane reforming
$n\text{-}C_5H_{12} + 5H_2O \rightarrow 5CO + 11H_2$	(15)	Steam n-pentane reforming
Reforming reactions		
$CO +2H_2 \leftrightarrow CH_4 + H_2O$	(16)	Steam methane reforming
$CO2 +H_2 \leftrightarrow CO + H_2O$	(17)	Water gas shift

Results and Discussion

Process Description and Simulation of Syngas to Methanol Unit

Methanol synthesis takes place at a temperature of 765 °C and a pressure of 111 bar with the Zn/Cu catalyst after producing reformed gas. Because of the equilibrium reactions, only a small amount of the compounds in the synthesis gas enter the reaction by passing through the catalyst bed, and the rest of the compounds leave the reactor unchanged. Therefore, for maximum methanol production, the methanol in the flaring gas must be separated, and the rest of the gas must be returned to the reactor as a return flow. The methanol synthesis cycle, which includes methanol separator drums, heaters, coolers, and synthesis reactors, is used for this purpose. According to Fig. 6, the reformed gas flow produced in the synthesis gas unit enters the compressor (K-100), increasing the gas pressure to 20 bar. After cooling in the coolers (E- 117, E102), this flow enters the separator (V-100). After that, the liquid and gas phases are separated in this separator, and the gas flow enters the compressor (K-101). In this compressor, the gas pressure is increased to about 149 to 150 bar, and before entering the methanol production reactor (ERV-101) in (E-103), the final heating is done. The methanol synthesis reactor is an equilibrium type. Methanol synthesis reactions are given in two equilibrium reactions, 7 and 8.

$CO_2 + H_2 \leftrightarrow CH_3\ OH + H_2\ O$ (7)

$CO + H_2\ O \leftrightarrow CO_2 + H_2$ (8)

Characteristics of reactor equilibrium reactions are illustrated in Table 6.

Process Description and Simulation of MTP Unit

The methanol flow coming out of the methanol production unit for heating after passing through the heat exchangers (E-101, E-102), its temperature is increased to 180 °C, and this flow enters the heater (E-102) with a temperature increase up to 390 °C.

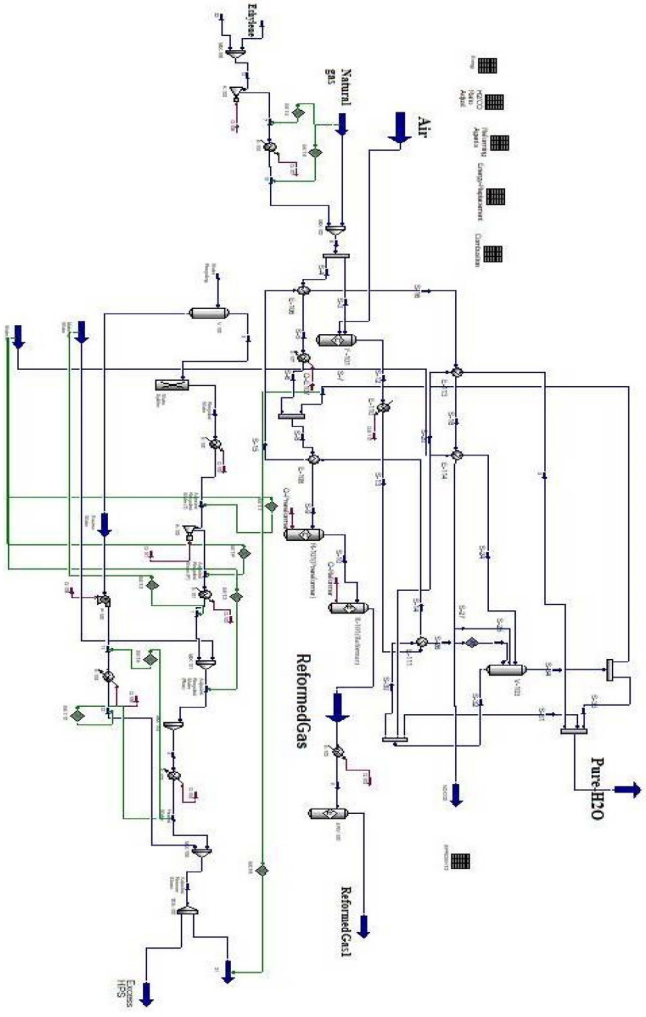

Fig. 6 Arrangement of synthesis gas production unit in Aspen HYSYS simulation media.

Table 6 Characteristics of reactor equilibrium reactions.

$CO_2 + H_2 \leftrightarrow CH_3OH + H_2O$ (20)							
T	Keq	T	Keq				
37.8	10-2× 9.116	482.2	10-7× 2.492				
93.3	10-3× 4.524	537.8	10-7× 1.213				
148.9	10-4× 4.463	593.3	10-8× 6.403				
204.4	10-5× 7.002	648.9	10-8× 3.620				
260	10-5× 1.529	704.4	10-8× 2.169				
315.6	10-6× 4.273	760	10-8× 1.366				
371.1	10-6× 1.442	815.6	10-9× 8.979				
426.7	10-7× 5.646						
T	Keq	T	Keq	T	Keq	T	Keq
93.3	4523	398.9	11.8	648.9	1.966	898.9	0.754
T	Keq	T	Keq	T	Keq	T	Keq
148.9	783.6	426.7	9.03	676.7	1.72	926.7	0.697
204.4	206.8	454.4	7.05	704.4	1.512	954.4	0.647
232.2	119	482.2	5.61	732.2	1.34	982.2	0.6037
260	72.75	510	4.55	760	1.202	1037.8	0.5305
278.8	46.70	537.8	3.749	787.8	1.08	1093.3	0.4712
315.6	31.44	565.6	3.13	815.6	0.9813	1148.9	0.4233
343.3	22	593.3	2.653	843.3	0.894	1204.4	0.2843
371.1	15.89	621.1	2.27	871.1	0.8192		

This flow is sent to the dimethyl ether (DME) equilibrium reactor (EVR-100) by the flow (Mixed Feed) after passing through the pressure relief valve and reducing the pressure to 8.5 bar.

The flow (Mixed Feed) after entering the reactor (EVR-100) causes a large amount of methanol to be converted into dimethyl ether according to the reaction (20). Due to the unavailability of the synthetic information of the methanol to dimethyl ether conversion reactor, an equilibrium reactor was used for simulation. The unavailability of detailed synthetic data on the DME to propylene conversion reactor caused the laboratory results of the DME to propylene conversion reactor to be used for the conversion percentage of the equilibrium reactions, and the conversion reactor was used instead of the plug reactor to convert DME to propylene. Therefore, the gas phase flow (to Conversion Reactor) output from the equilibrium reactor (EVR-100) with a temperature of 483 °C and P=5.8 bar enters the conversion reactor (CVR-100). After the reaction, the product flow (Wet Propylene) is removed. The output flow from the reactor (Wet Propylene) enters the splitter tower (X-100) for separation. The pure water flow is separated from the bottom of the tower, and the rest of the gas flow (Mixed Propylene) is separated from the top of the tower. The gas flow (Mixed Propylene) enters the splitter tower (X-100) to separate and purify propylene. Thus, the pure flow of propylene is separated from the bottom of the tower (M-11), and the flow rich in ethylene is separated from the tower top. Table 7 shows the equilibrium reactions of the DME to propylene conversion reactor and the conversion percentage of each reaction.

$$2CH_3OH \leftrightarrow CH_3OCH_3 + H_2 \quad (9)$$

Process Description and Simulation of the Integrated NG to Poly Propylene Process (NGTP Plant)

Considering that the goal of this process simulation and optimization is to increase the production of propylene in the integration arrangement. Waste gases from the methanol, MTP, and syngas units are returned to the syngas and methanol units for recovery. In this process, according to Fig. 7, the gas flow from the reactor (F-101), which is used to supply the energy required by the reformer gas equipment, after supplying the necessary energy to the equipment, produces a flow that is rich in N_2 and CO_2.

This stream enters the splitter tower (X-100) for recovery and leaves the carbon dioxide (CO_2) tower and the nitrogen and water mixed flow (N_2-H_2O) from the bottom of the tower. Then, this stream enters the splitter tower (X-101). In this tower, N_2 is separated from the top, and H_2O is separated from the bottom. The carbon dioxide stream separated from the splitter (X-100) named (CO_2) is mixed with the carbon dioxide stream separated in the methanol unit and enters the methanol synthesis reactor to participate in the reaction. The ethylene stream separated in the MTP unit is sent to the synthesis gas unit for recovery.

Process Description of the PTPP Unit

Because of the lack of polymer compounds and a suitable polymerization kinetic package, it is impossible to simulate a polymer system by Aspen HYSYS. Aspen Plus-V11 has been used to simulate the PTPP unit.

According to Fig. 8, the input feed to this process is the propylene product obtained from the MTP process simulated in Aspen HYSYS. Thus, after mixing, the C_{3Feed} stream includes propylene within the N_2 and H_2 streams that enter the CSTR reactor. This process uses a $TiCl_4$ catalyst reinforced on Triethylaluminium (TEAL).

Table 7 DME to propylene reactions.

Reaction stoichiometric relations	Conversion (%)
$CH_3OCH_3 \rightarrow C_2H_4$	96.61
$CH_3OH\ C_2H_4 + H_2O$	73.81
$CH_3OCH_3 + C_2H_4CH_3OH + C_3H_6$	33.14
$CH_3OH + C_2H_4 \rightarrow C_3H_6 + H_2O$	73.17
$C_3H_6 + CH_3CH_3 \rightarrow C_4H8 + CH_3OH$	34.74
$C_3H_6 + CH_3OH \rightarrow C_4H_8 + H_2O$	56.59
$C_4H_8 + CH_3OCH_3 \rightarrow C_5H_{10} + CH_3OH$	66.81
$CH_3OHCO + 2H_2$	29.28
$CO + H_2O \rightarrow CO_2 + H_2$	46.24
$CH_3OH + H_2 \rightarrow CH_4 + H_2O$	25.20
$C_2H_4 + H_2 \rightarrow C_2H_6$	66.10

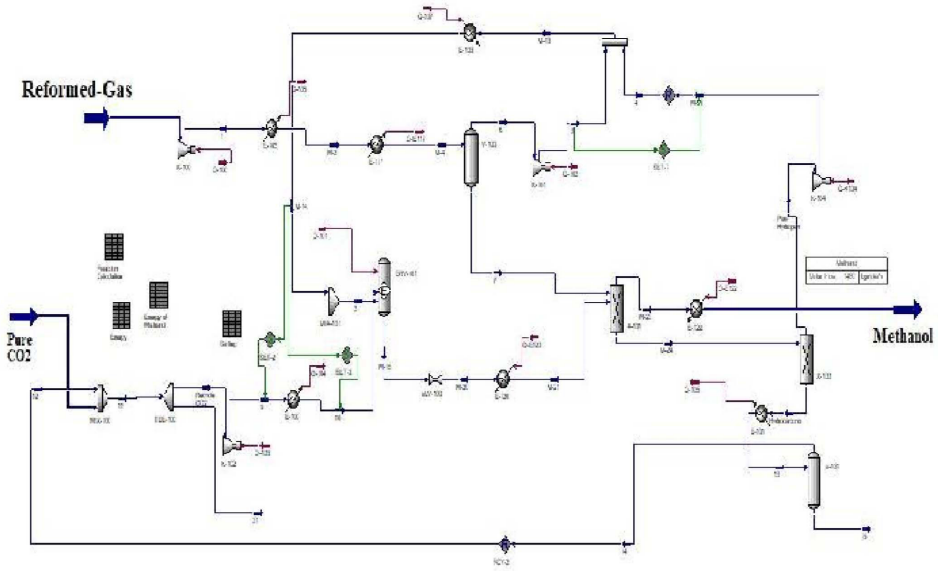

Fig. 7 Arrangement of methanol unit in Aspen HYSYS simulation media.

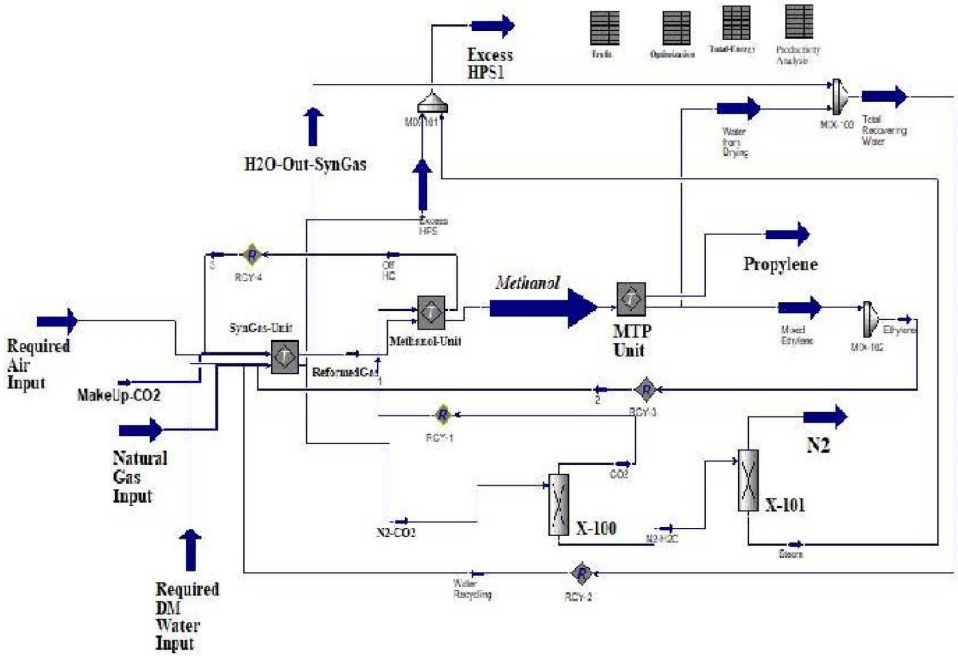

Fig. 8 Simulation arrangement of the integrated NG to propylene (NGTP).

In this process, the amount of $TiCl_4$ catalyst with a specific ratio $(6.763\times10^{-5}) \times (C_{3Feed})^2$ is used. Therefore, the flows with the catalyst after entering the reactor and performing the reaction. The vapor stream comes out from the top, and the polymer stream comes out from the bottom of the reactor. The discharged polymer stream, which is rich in polypropylene polymer, enters the separator (STRIP1) for separation, and the unreacted propylene stream (GAS1) comes out from the top flow (POWDER2). The stream (POWDER2) enters the separator (STRIP2) for separation, and the stream rich in nitrogen exits from the top of the tower. The desired product, i.e., polypropylene (PP-PROD), exits from the bottom of the tower. An overview of the simulated PTPP process in Aspen Plus has been presented in Fig. 9.

Optimization Algorithm: SCA

Due to its simplicity and less tedious parameter tuning over other multi-agent-based optimization algorithms, Sine Cosine Algorithm (SCA) has gotten lots of attention from numerous researchers for resolving optimization problems [37]. SCA has attracted great attention from researchers and has been widely used to solve optimization problems in several fields. This attention is due to its reasonable execution time, good convergence acceleration rate, and high efficiency compared to several well-regarded optimization algorithms in the literature. This manuscript briefly overviews the basic SCA and its variants divided into modified, multi-objective, and hybridized versions [38]. Sine Cosine Algorithm is a recently developed algorithm based on the characteristics of sine and cosine trigonometric functions to solve global optimization problems [39]. The SCA is a recently developed meta-heuristic algorithm based on the mathematical characteristics of sine and cosine trigonometric functions. This algorithm was designed by Mirjalili in 2015 [40]. Like other population-based meta-heuristic optimization algorithms, SCA also starts with a set of randomly distributed solutions. Then, each solution updates its position with the help of the following equations:

$$x_{i.t+1} = \begin{cases} x_{i.t} + A\sin(r1) \mid Cxbest - x_{i.t} \mid & \text{if } r < 0.5 \\ x_{i.t} + A\cos(r1) \mid Cx_{best} - x_{i.t} \mid & \text{otherwise} \end{cases} \quad (11)$$

where $x_{i.t}$ and $x_{i.t+1}$ represent the i^{th} solution vector at t^{th} and $(t+1)^{th}$ iteration, respectively, x_{best} is the fittest solution in the solution set, r parameter is a uniformly distributed random number in the interval (0, 1), r_1 is a vector that decides the direction of the moment of the current solution, which can be either towards the x_{best} or outside x_{best}. The vector C provides weight to x_{best}, which emphasizes the exploration ($C > 1$) and exploitation ($C < 1$). The vector C also helps avoid premature convergence at the end of iterations. The vector C helps in the transition from sine to cosine functions and vice versa. The effect of random number A on sine and cosine functions is shown in Fig. 10.

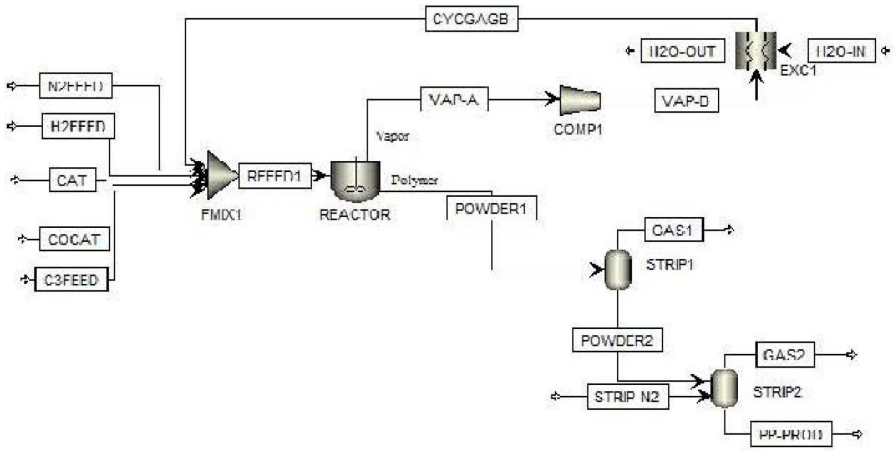

Fig. 9 Overview of simulated PTPP process in Aspen Plus.

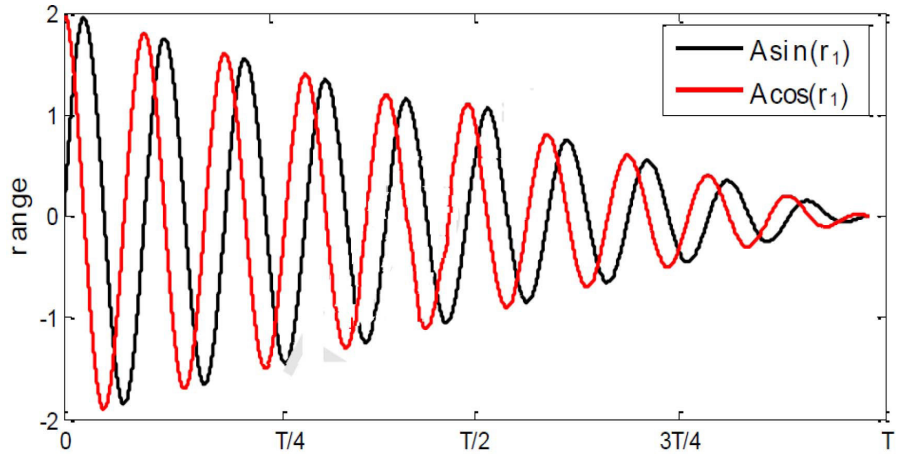

Fig. 10 The impact of sine and cosine functions with random vector *A*.

The parameter A is a random vector that decides the area of the search space around the current solution. This region of search space may lie inside the x_{best} and $x_{i.t}$ or outside them. The parameter A also helps in the exploration and exploitation of a search space and in maintaining a suitable balance between them. In the first half of the total number of iterations, coefficient A contributes to exploring a search space. In contrast, the second half of the total number of iterations is devoted to exploiting an available search space. Mathematically, the vector A can be defined as follows:

$$A=2-2(t/T) \quad (12)$$

where T represents the maximum number of iterations predefined as a termination criteria for SCA. The steps of the Sine Cosine Algorithm are pointed out in Algorithm 1.

	Algorithm 1. Classical Sine Cosine Algorithm (SCA)
1	Generate the uniformly distributed initial set of random solutions within the search space.
2	Compute the fitness of each solution vector.
3	Initialize the parameters T (maximum number of iterations) and coefficient A.
4	Select the fittest solution x_{best} from the set of solutions.
5	Initialize the iteration count $t = 0$
6	while $t < T$
7	Update each solution vector with the help of Equations (7) and (8).
8	Compute the fitness of each updated solution vector.
9	Update the best solution .
10	Update the coefficient A.
11	$t = t + 1$
12	end of while
13	Return the fittest solution .

Although the sine cosine algorithm is very efficient in exploring the search space in many cases, it suffers from some significant difficulties, like skipping accurate solutions and local optima stagnation. Therefore, an improvement is required in the search strategy of SCA. The present work attempts to improve the efficiency of classical SCA.

Algorithms based on a random population start optimizing the process using random solutions that are not guaranteed to reach the characteristic objective function in one optimization step. However, repeating random solutions and optimization steps and checking multiple solutions obtained for the objective function. The best optimal solution can be achieved. With all the differences between the population-based optimization algorithms, the optimization processes in all of them are performed in two stages:

1) Exploration Phase
2) Exploitation Phase

In the exploration phase, the optimization algorithm combines a set of random solutions to find the best region of the search space. In the exploitation phase, changes in random solutions are done gradually, and the steps in exploration are much more than random changes.

Equations 22 and 8 show the position update in the SCA algorithm.

The SCA optimization algorithm can optimize the problem using the reasons mentioned below [41]:

• In the SCA algorithm, after creating random solutions for the system to be optimized, it starts to improve these solutions, thus preventing the creation of a local optimum based on one solution, and the number of discoveries increases.

• The search space increases by increasing and decreasing the sine and cosine function values from 1.0 and -1.0, respectively.

• When the return value of sine and cosine is between -1 and 1, promising regions of the search space are explored.

• Changing the SCA algorithm's adaptive range of sine-cosine functions makes it easy to reach from exploration to exploitation.

• The best optimal solutions approximated in the optimization are stored as the destination and are never lost during the optimization.

• In this algorithm, the solutions constantly update their position concerning the best solution obtained until they choose the best search spaces during optimization.

• Considering the black box optimization problem in the SCA algorithm, it can be used in many fields subject to proper formulation.

Simulation and Optimization Results of MTP and PTPP Units

In this study, maximization of the PP productivity while maintaining the quality of the polymer is considered the primary goal (objective function). Aspen HYSYS and Aspen Plus simulate the MTP and PTPP units, respectively.

The output or product of the MTP unit is the feed or input of the PP unit. As a result, with the increase in the MTP unit's productivity, the PP unit's productivity will increase. Due to the large number of parameters that can be changed and affect the manufactured product, using the sensitivity analysis of Aspen HYSYS and Aspen Plus, the parameters affecting the manufactured product were examined, and the most important parameters were selected as decision variables for the optimization problem.

In engineering processes, parameters such as energy consumption reduction, equipment cost reduction, productivity increase, etc., are selected as the objective function, and optimization is performed on these parameters.

There are various optimization methods depending on the objective function type and problem type [42]. Each of the optimization methods has its advantages and disadvantages [43]. Most optimization methods perform an initial guess near the local optimal objective function. In addition to the inaccuracy of the general answer, these methods also have problems, such as an exponential increase in the calculation time by increasing the parameters of the problem and the assumptions that these methods make according to the type of problem, which are not correct most of the time. Also, these methods need to be modified depending on the type of objective function.

New optimization methods and algorithms, called metaheuristic methods, were created to solve these problems. These methods are not defined for a specific type of problem and are general methods [44].

Metaheuristic means to understand, know, and explore [45]. In these algorithms, the search for the optimal solution is based on probability and randomly. For this reason, these algorithms are also called random algorithms. Due to the importance of optimization in processes, the number of these algorithms is gradually increasing. The most famous, modern, and widely used of these algorithms are the pointing genetic algorithm (GA), particle swarm optimization (PSO), simulated annealing (SA), ant colony (AC), artificial bee colony (ABC), dragon-fly algorithm (DA), and sine cosine algorithm (SCA).

In this study, for the optimization of an integrated GTPP plant, SCA has been used.

For this step, integration and linking of Aspen HYSYS with Aspen Plus must occur to check all variables simultaneously. On the other hand, SCA is an optimization code provided in MATLAB. Therefore, a hybrid between Aspen HYSYS, Aspen Plus, and MATLAB should be done by connecting these three software.

Fig. 11 presents a schematic diagram of Aspen HYSYS, Aspen Plus, MATLAB, and transferring data between them. The specifications of NG to PP plant output for the basic state, including syngas, methanol, propylene, and polypropylene subunits, obtained from the simulation of these units by Aspen HYSYS and Aspen Plus, are shown in Table 8.

Sensitivity Analysis of Integrated Process in Aspen HYSYS and Aspen Plus

Sensitivity analysis is a tool to show the output response of a process by changing the key variables in the process.

According to this feature, it is possible to check the effect of each parameter separately by changing one or more parameters. Considering this feature, changing the proposed parameter for further investigations in the optimization field is possible. The objective function in the Aspen HYSYS is the productivity maximization of propylene production in the MTP. The parameters that affect the objective function are a) the temperature of the methanol production, b) the reformer gas temperature, c) the methanol reactor pressure, and d) the ratio of recovered CO_2 recycled to the methanol reactor. After analysis, the results are given in the results section.

After examining the influencing parameters in the MTP unit by the Aspen HYSYS, the influencing parameters in the propylene to polypropylene unit in the Aspen Plus were investigated, which is the function of the goal of increasing the polypropylene product. The influencing parameters in the objective function are a) the temperature of the input feed to the propylene-to-polypropylene reactor and b) the ratio of the titanium tetrachloride catalyst to the input feed. Analysis results of which are given in the result section.

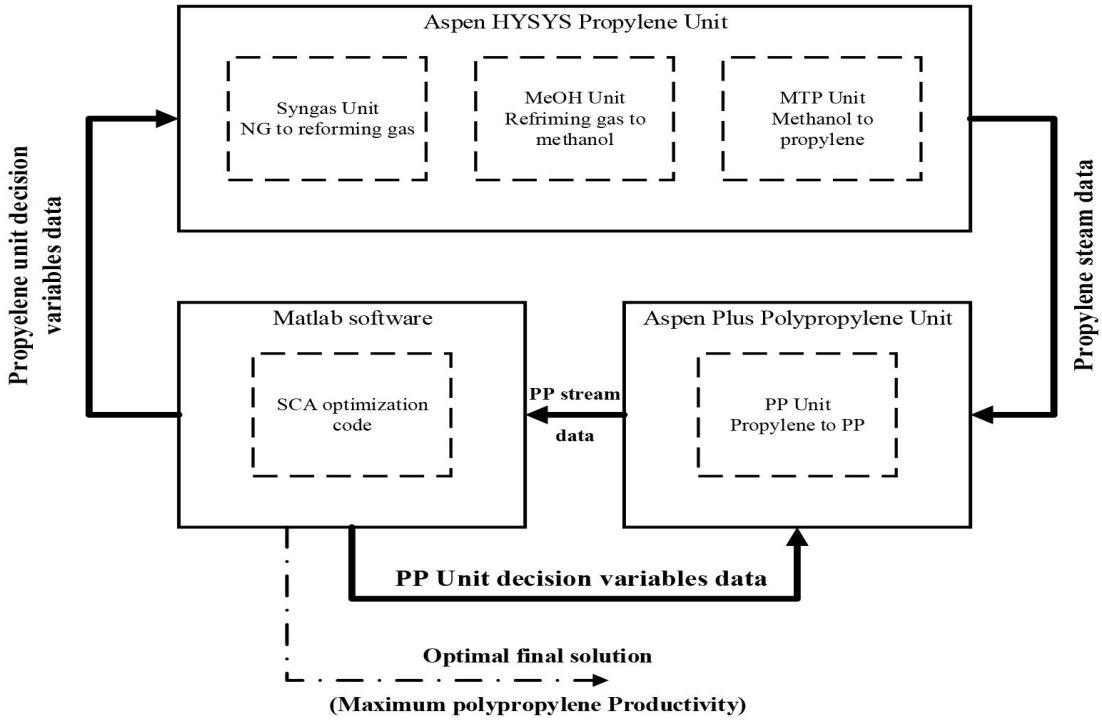

Fig. 11 Schematic diagram of linking between simulation and optimization boxes.

Table 8 Results of integrated GTPP plant simulation.

Reformed gas stream properties	Propylene stream properties		
Variable	Value	Variable	Value
T	600 °C	T	792 °C
P	7.4 bar	P	1.013 bar
Mole (%)			
CH_4	0.84	CH_3OH	0.00
C_2H_6	0.00	DME	0.00
H_2O	17.5	C_2H_4	0.00
H_2	60.80	H_2O	0.00
CO	16.28	H_2	0.00
CO_2	3.52	CO	0.00
O_2	0.00	CO_2	0.00
N_2	1.07	C_3H_6	1
Mass flow (ton/h)	513.30	Mass flow (ton/hr.)	12.323
Volume flow (m^3/h)	717.40	Volume flow (m3/hr.)	23.65
Methanol stream properties	Polypropylene stream properties		
T	29.67 °C	T	60 °C
P	28.61 bar	P	1.0 bar
Mole (%)			
CH_4	0.00	$TiCl_4$	4.092E-03
C_2H_6	0.00	TEA	0.057
H_2O	0.09	C3H6	0.169
H_2	0.00	PP	99.75
CO	0.00	H_2	8.23E-8
CO_2	1.00	N_2	0.011
CH_3OH	98.91	H_2O	0.00
Mass flow (ton/hr.)	46.68	Mass flow (ton/h)	16279.66
Volume flow (m3/hr.)	58.63	Volume flow (m^3/h)	0.02

Results of Sensitivity Analysis

The most important product in the MTP process is propylene, and in the PP process, polypropylene. Sensitivity analysis or case study is an option in Aspen HYSYS and Aspen Plus, which was used to analyze the parameters affecting the productivity of propylene and polypropylene.

The feed flow has been kept constant during the investigation of these changes. In the MTP and PP process simulation, the changes of effective parameters on the two main product productivity as the objective function of the optimization step have been investigated.

The operating parameters examined are as follows:

- Production temperature of reformer gas ($T_{Ref.gas}$)
- Methanol production temperature in the methanol unit (T_{MeOH})
- Pressure of the methanol synthesis reactor in the methanol unit (p_{MeOH})
- Ratio of hydrocarbon return flow rate to methanol synthesis reactor (R_{HC})
- Temperature of the input feed to the polypropylene production reactor (T_{PPR})
- PP reactor pressure on PP productivity (P_{PPR})
- Ticl4 mass flow on PP productivity (MF_{Ticl4})
- TEA mass flow on PP productivity (MF_{TEA})

Effect of T($R_{ef.gas}$) on Propylene Productivity

The reformer temperature is the first operating parameter affecting the propylene as one main product of an integrated simulated plant that has been investigated. As seen in Fig. 12, with the increase in temperature between 710 to 930 °C, the productivity of propylene rises. As a result, the temperature of the reformer is one of the most influential parameters that, with its changes, propylene productivity is changed. However, the question is about the range of changes considered for this variable. Based on this route's studies and operational limitations, the temperature between 700 °C and 950 °C seems more reasonable. The most important factor that changes the propylene productivity at different temperatures is the composition of the synthesis gas production and the ratio of hydrogen to carbon monoxide (H_2/CO) in this product, which also affects the amount of propylene production.

Effect of T_{MeOH} on Propylene Productivity

The temperature of the methanol production reactor in the methanol unit is the second effective operating parameter investigated. Considering the reaction of methanol, which is an exothermic reaction, if the temperature increases, the heat produced in the system will also increase, and by consuming this heat, the system will try to advance the reaction to the left side and thus lead to less methanol production.

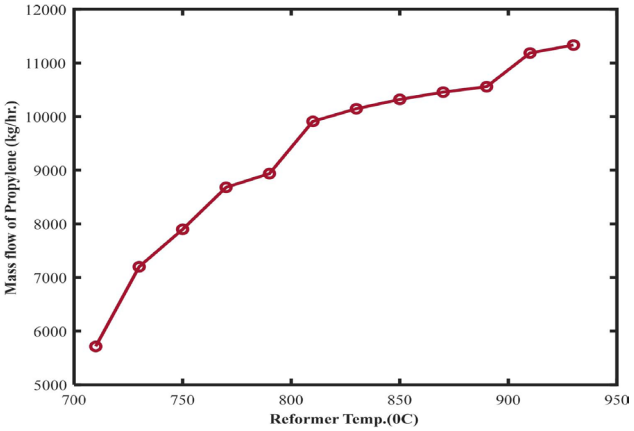

Fig. 12 Effect of reformer temperature on propylene productivity.

If this reaction is performed at a lower temperature, more methanol will be produced, but this decrease in temperature will also decrease the reaction rate. Therefore, in practice, this temperature should be set to an optimal level so that methanol production has a suitable amount in a certain period. Fig. 13 shows the changes in the temperature of the methanol synthesis reactor. By increasing the temperature from 200 to 300 degrees Celsius, the amount of the final product in the MTP unit, i.e., propylene, has decreased. As the temperature of the methanol synthesis reactor increases, the amount of methanol produced will drop, reducing production capability and the percentage of conversion to products.

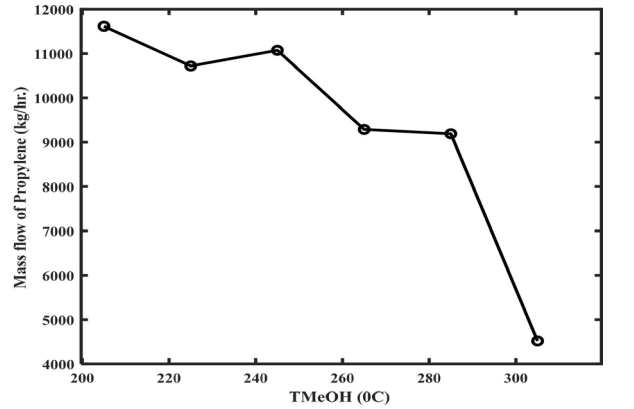

Fig. 13 Effect of methanol temperature on propylene productivity.

Effect of P_{RMeOH} on Propylene Productivity

The effect of methanol reactor pressure on propylene productivity is shown in Fig. 14. According to Lochatelier's principle, with the increase in pressure caused by the decrease in volume, the equilibrium moves towards having fewer moles. On the contrary, with the increase in volume, the system will experience a decrease in pressure, and its progress will be in the direction where the number of moles is higher. If the number of moles of gas is the same on each side of the reaction, changing the pressure will not affect the equilibrium. According to the relationship of methanol productivity, as can be seen, by increasing the reactor pressure from 70 bar to 160 bar, the progress of the reaction is toward fewer moles, that is, the production of the final product of propylene. By increasing the pressure, the conversion percentage of the methanol synthesis reactor has increased, which increases the amount of methanol produced and, as a result, increases the final product of propylene.

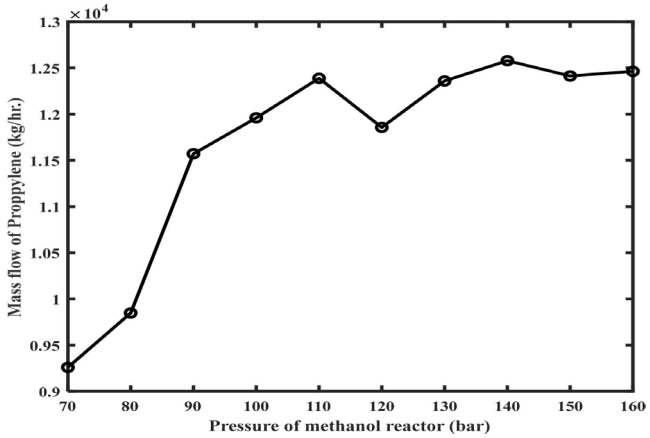

Fig. 14 Effect of methanol reactor pressure on propylene productivity.

Effect of recycle ratio of off-gas to methanol unit on propylene productivity

Fig. 15 represents the influence of the hydrocarbon return flow ratio to the methanol synthesis reactor changing on propylene productivity. By increasing the ratio from 0.0 to 0.8, the mass flow of propylene increases, and from 0.8 to 1.0, the value of this variable decreases. As a result, from 0.0 to 0.8, the reactor conversion and the productivity of methanol production increases. Therefore, the productivity of propylene increases. In the range of 0.8 to 1.0, the conversion in the reactor is reduced, which reduces the propylene productivity.

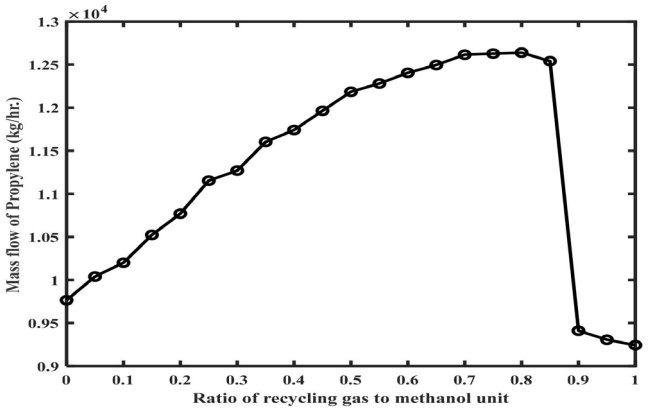

Fig. 15 Effect of recycling gas ratio to methanol unit on propylene productivity.

Effect of PP Reactor Temperature on PP Productivity

Fig. 16 illustrates the PP reactor temperature on the polypropylene productivity as the plant's final product. According to the figure, it can be seen that the mass flow rate of polypropylene production increases up to a temperature of approximately 60 °C and then decreases. Therefore, an optimal temperature must be selected for the operating condition of this plant. The increase in product production can be because the main reaction is endothermic, which causes the reaction to increase with the increase in temperature. After reaching the optimum temperature, the temperature increase does not affect the increase in production.

Effect of PP Reactor Pressure on PP Productivity

Fig. 17 shows the PP reactor pressure on the polypropylene productivity. As the behavior in the figure shows, the pressure fluctuates in the production rate of polypropylene. Therefore, since there is no fixed behavior, it is necessary to choose this variable to calculate the best value in optimization.

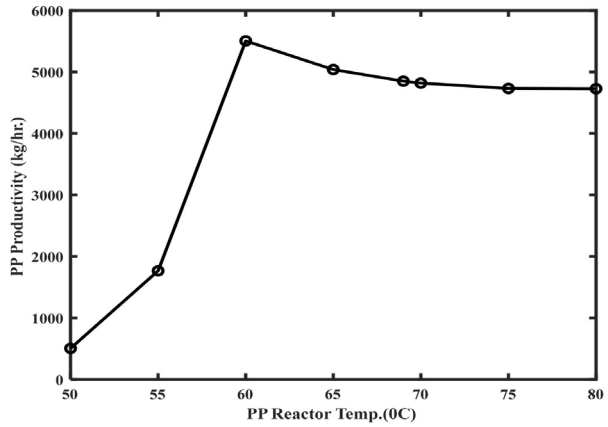

Fig. 16 Effect of PP reactor temperature on PP productivity.

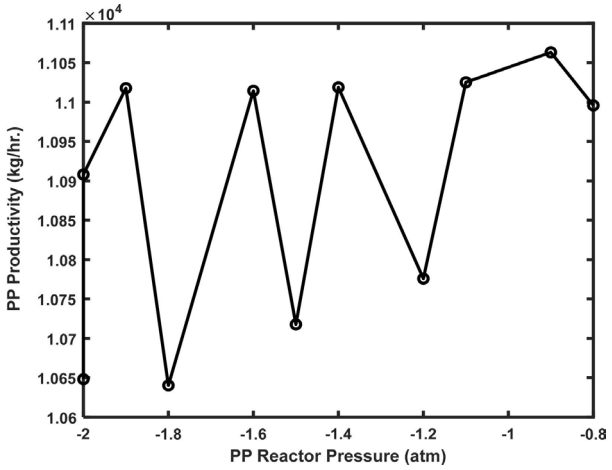

Fig. 17 Effect of PP reactor pressure on PP productivity.

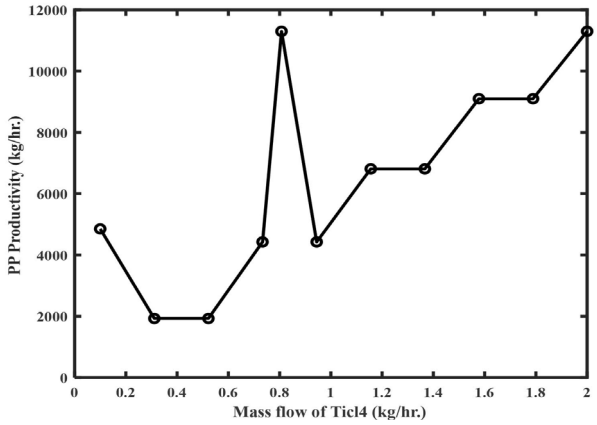

Fig. 18 Effect of $Ticl_4$ Mass Flow on PP Productivity.

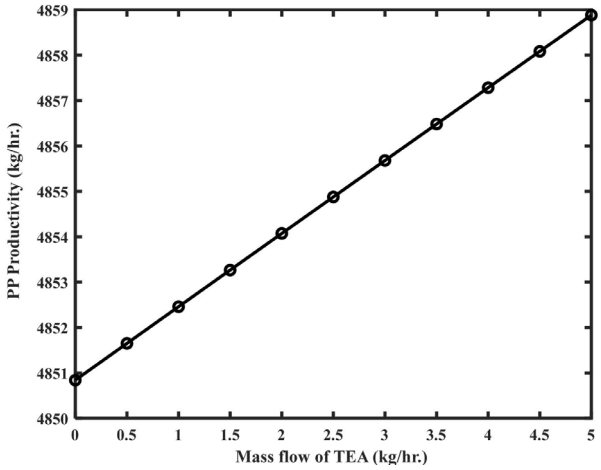

Fig. 19 Effect of TEA mass flow on PP productivity.

Effect of CAT Stream Mass Flow on PP Productivity

According to Fig. 18, the mass flow rate of produced polypropylene oscillated with the increase in the $Ticl_4$ catalyst mass flow rate. On the other hand, due to the high price of this catalyst, the use of this material may not be economical. Therefore, in the optimization step, a tradeoff between the price of the catalyst and growth income due to increasing PP productivity should occur.

Also, this figure represented the maximum PP productivity at 0.8 kg/h of Ticl4 mass flow.

Therefore, an optimal point of these decision variables will be available in the optimization step.

Effect of COCAT Stream Mass Flow on PP Productivity

Based on the results obtained from the effect of changes in TEA mass flow on PP productivity (Fig. 19), it can be seen that with the increase in TEA mass flow, PP productivity also increases.

However, it should be noted that these changes are minimal, from 4851 kg/h to 4859 kg/h, which can be ignored

This trend of $Ticl_4$ mass flow effect on PP productivity seems usual.

Because the behavior of the polymerization reactor versus most variable variations, such as temperature, pressure, and flow, is nonlinear, we cannot explain the main reason for this trend. On the other hand, catalysts and reactions may mainly cause this trend.

Effect of TPPR, PPPR, CAT, and COCAT Streams Mass Flow on MWN Property of PP

Polymers consist of repeat units (monomers) chemically bonded into long chains. Understanding the physical properties of a polymer (such as mechanical strength, solubility, and brittleness) requires knowledge of the length of the polymer chains.

Chain length is often expressed in terms of the molecular weight of the polymer chain, related to the relative molecular mass of the monomers and the number of monomers connected in the chain. However, all synthetic polymers are polydisperse because they contain unequal-length polymer chains, so the molecular weight is not a single value. The polymer exists as a distribution of chain lengths and molecular weights. Therefore, the molecular weight of a polymer must be described as some average molecular weight calculated from the molecular weights of all the chains in the sample. This overview describes the commonly used molecular weight averages determined by gel permeation chromatography (GPC) and size exclusion chromatography (SEC), their definition, and the classical methods initially used to measure them. The number average molecular weight is the statistical average molecular weight of all the polymer chains in the sample and is defined by:

$$M_n = \frac{\sum M_i N_i}{\sum N_i} \quad (13)$$

where N_i is the number of chains with M_i molecular weight. M_n can be predicted by polymerization mechanisms and

is measured by methods that determine the number of molecules in a sample of a given weight; for example, colligative methods such as end-group assay. If M_n is quoted for molecular weight distribution, there are equal numbers of molecules on either side of M_n distribution.

Based on the results, the following factors affect the MWN differently. Based on Fig. 20, except for the pressure increase factor (as seen in Fig. 21(C)), other items (Fig. 20(A), Fig. 20 (B), and Fig. 20(D)) decrease the MWN by increasing. It means that all effective variables must be considered in the optimization process to achieve the best and most optimal solution.

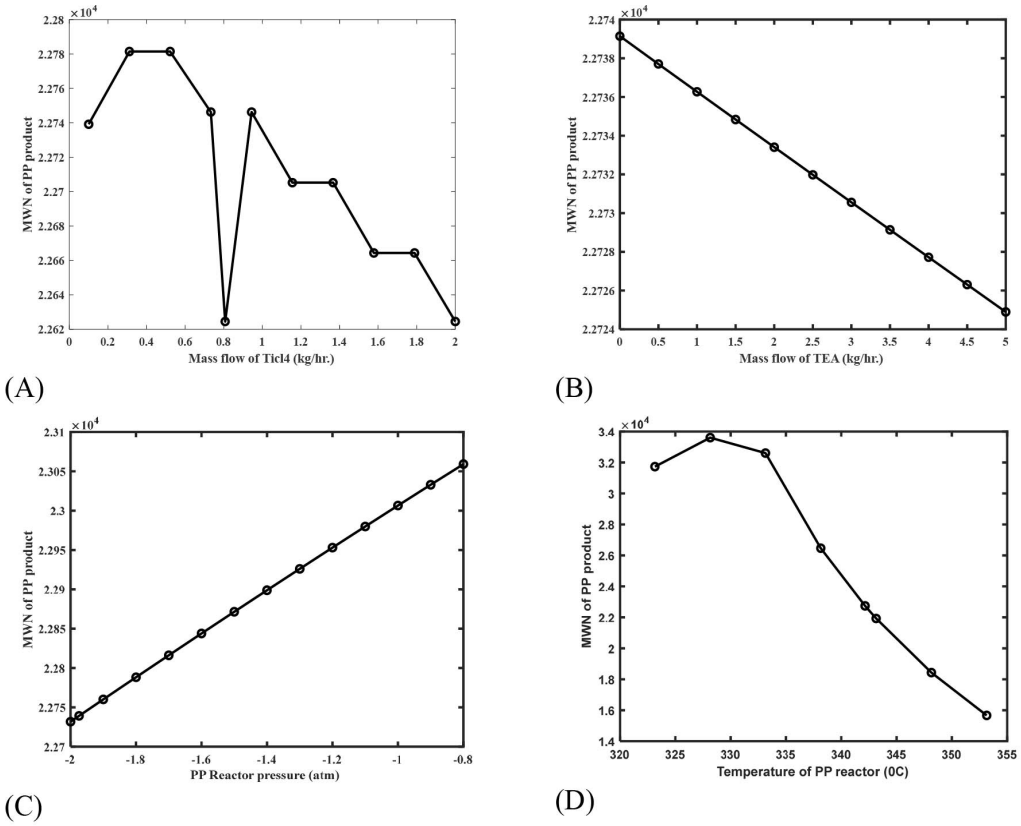

Fig. 20 Effect of all studied parameters on MWN of PP product (A to D).

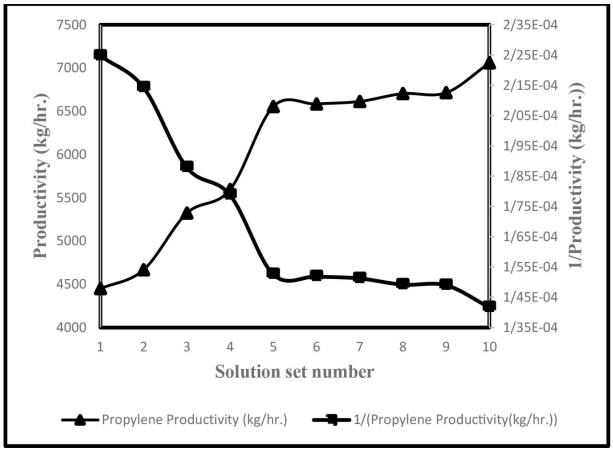

Fig. 21 The optimal solutions obtained for the optimization problem after performing 40 stages of population generation for the decision parameters.

Optimization of Studied GTPP Plant

Optimization Problem Formulation

One investigation in this study is recycling an unreacted gas stream entitled "Recycle Gas". This stream contains mainly H_2, CO, and CO_2 components. The recycled stream is directed to the methanol unit.

As the target is productivity improvement, a split ratio of "Recycle Gas" between the methanol unit and venting was selected as the decision variable for optimization, and the total product of the integrated propylene process was selected as the objective function.

In all cases, input natural gas's total mass flow rate remains constant (35368 kg/h).

The objective functions were optimized by fulfilling the following constraints (Equations 2 and 3). Thus, the optimization problem can be expressed as follows (2-6):

Maximize PP productivity (kg /hr.) (Maximize polypropylene

Process Products) (14)
780 °C ≤x_1=$T_{Ref.gas}$≤850 °C (15)
230 °C ≤x_2=T_{MeOH}≤280 °C
0 ≤x_3=R_{HC}≤1.0 (split ratio=(Mass flow of recycled gas to methanol unit)/(Total Mass flow of recycled gas)) (16)
110 bar≤x_4=P_{MeOH}≤150 bar (17)
58 °C ≤x_5=TPPR≤63 °C (18)
-2 atm. ≤x_6=PPPR≤-0.8 atm. (19)
0.1 kg/hr. ≤x_7=MF_{Ticl4}≤2 kg/hr. (20)
0.0 kg/hr. ≤x_8=MF_{TEA}≤5 kg/hr. (21)
Constraints:
3.5≤x_7= (H_2/CO) mole basis at reformed gas≤4.0 (22)
x_8=Methanol purity at methanol stream (%) ≥98 (mole basis) (23)
x_9=Propene purity at C_3 stream (%)≥99 (mole basis) (24)
x_{10}=Polypropylene purity at PP stream (%)≥99.8 (mole basis) (25)
x_{11}=MWN of PP stream≥2.0 (26)

Optimization Results

The SCA algorithm method has been used for optimization to produce a set of optimal solutions. Optimization is done using the population number of 20. Additional input information to the SCA algorithm optimization program is given in Table 9.

In the single objective optimization of NG to PP unit simulation, if the range of decision parameters is according to Table 10, three problems arise. 1). Due to the extensive search space size, each parameter's defined interval must be changed for optimization. If the defined range for parameters is large in this case, Aspen HYSYS and Aspen Plus may have convergence problems, and the connection between optimization with MATLAB and simulation will be broken. The reason for this problem is the recycles in the unit, the splitters in the simulation, the adjusting function, etc.

2) Processing large intervals is very time-consuming. Suppose these processes run into convergence problems in Aspen HYSYS and Aspen Plus after a few days, and the connection with MATLAB is interrupted. In that case, it is forced to rerun these steps from the beginning, which causes a waste of time.

3) Processing large intervals requires powerful computing systems.

To solve this problem, according to the sensitivity analysis, the interval in which the most changes occur was selected according to Table 10.

Table 9 Additional input information to the SCA algorithm optimization program.

Parameters topic	Value
Number of decision variables	8
Number of constraints	5
Objective function	1
Population size	20
Maximum number of production	40

In Table 11, the values of optimal decision-making variables are obtained using the integrated Aspen HYSYS-SCA algorithm for the natural gas to propylene process. In this step, maximization of propylene mass flow is considered the objective function. It noted that propylene is the main feed of the PP unit, so by increasing the productivity of MeOH, PP productivity increases, too.

Table 12 shows the optimal solution obtained for the optimization problem of natural gas to propylene plant after performing 40 stages of population generation for the decision-making parameters compared to the base case simulated parameters. According to this table, propylene productivity as an objective function of this plant increased from 11,318 to 12,723 kg/hr. (about +12%).

Table 13 presents the optimal propylene values for polypropylene plant decision variables gained using the integrated Aspen Plus-SCA algorithm.

Maximization of polypropylene mass productivity (PPP) is the objective function of this unit and overall plant. TPPR, PPPR, M_{FTicl4}, and M_{FTEA} are the decision variables.

The definition of M_{FTicl4} and M_{FTEA} variables is indicated in Table 13:

MFTicl4: Total mass flow of Ticl4 stream.

In this table, the mass composition of CAT and COCAT streams has been indicated. The CAT stream has three components ($Ticl_4$, C3H6, and C_3H_6). In the optimization formula, the CAT stream's total mass flow has been considered a decision variable. Because the COCAT stream has only a TEA component, by changing the total mass flow of the COCAT stream directly, the mass flow of TEA changes. The mass composition of all components in these two streams is fixed in all optimization cases.

Table 10 Final parameters to optimize the objective function.

Decision parameter	Parameter symbol	Variable math name	Lower limit	Upper limit
First step of optimization (natural gas to methanol); objective function = propylene productivity				
Reformed gas temperature (°C)	$TR_{ef.gas}$		780	850
Methanol reactor temperature (°C)	TM_{eOH}		230	280
Split ratio of hydrocarbon stream to methanol unit	R_{HC}		0.3	0.7
Methanol reactor pressure (bar)	P_{MeOH}		110	150
Second step of optimization (propylene to polypropylene); objective function = polypropylene productivity				
Polypropylene reactor temperature (°C)	T_{PPR}		58	63
Polypropylene reactor pressure (atm.)	P_{PPR}		-2 atm.	-0.8 atm.
Mass flow of CAT to Polypropylene reactor (kg/hr.)	M_{FTicl4}		0.1	2
Mass flow of COCAT to Polypropylene reactor (kg/h)	M_{FTEA}		0.0	5

Table 11 The optimal decision variable values obtained by the SCA algorithm.

Run No.	Decision variables	Objective function				
	$T_{Ref.gas}$	T_{MeOH}	RHC	P_{MeOH}	Min. 1/(Propylene productivity)	Max. Propylene productivity
1	780.91	277.35	0.67	12814.27	1.09×10-4	9187
2	699.87	277.33	0.33	13823.50	1.66×10-4	6021
3	753.54	288.20	0.31	10742.89	1.34×10-4	7479
4	738.84	279.20	0.35	15245.24	1.32×10-4	7583
5	875.53	225.91	0.70	14086.92	7.86×10-5	12723
6	793.12	192.11	0.22	14702.38	1.28×10-4	7807
7	822.15	282.44	0.73	13808.30	7.97×10-5	12541
8	913.91	229.95	0.54	15279.19	9.07×10-5	11030
9	750.18	230.75	0.28	12399.46	1.09×10-4	9149
10	813.01	256.07	0.38	13757.84	9.24×10-5	10817
11	819.39	279.00	0.42	12463.79	9.10×10-5	10984
12	877.83	241.89	0.68	14677.37	8.16×10-5	12259
13	766.84	259.97	0.57	1548.51	1.12×10-4	8943
14	759.19	240.99	0.21	14255.67	8.58×10-5	11658
15	812.10	265.65	0.55	13880.74	9.28×10-5	10772
16	815.77	294.44	0.34	13155.64	9.51×10-5	1517
17	862.63	285.63	0.42	16618.26	8.53×10-5	11724
18	847.37	238.15	0.43	13068.32	8.35×10-5	11969
19	723.98	229.48	0.52	13714.63	1.45×10-4	6876
20	822.23	257.63	0.36	14069.88	9.15×10-5	10926
Optimal point	875.53	225.91	0.70	14086.92	7.86×10-5	12723

Table 12 Comparing the optimal solution and simulated base case for the optimization of natural gas to propylene plant.

Decision variables and Objective function	Variable symbol	Simulation value	Optimization value	Changing (%)*(increasing (+), decreasing (-))
$T_{Ref.gas}$ (°C)		825	875.53	+6%
T_{MeOH}(°C)		250	225.91	-10%
R_{HC} (unitless)		0.5	0.7	+40%
P_{MeOH} (kPa)		12500	14086.92	+13%
1/(Propylene productivity (kg/hr.))		8.83×10^{-5}	7.86×10-5	-12%
Productivity of Propylene (kg/hr.)		11318	12723	+12%
$\text{Changing}(\%)=\frac{(\text{Simulation value-Optimization value})}{\text{Simulation value}}\times100\%$				

Table 13 Detailed definition of M_{FTicl4} and M_{FTEA} decision variables, and comparing optimal solution and simulated base case for the optimization of propylene to polypropylene plant.

Mass composition of CAT stream				
Component Name	$Ticl_4$	C_3H_6	C_3H_8	
	0.01	0.988	0.002	
Mass composition of COCAT stream				
Component Name	TEA			
Mass fraction	1.00			
Decision variables and objective function	Variable symbol	Simulation value (Base state)	Optimization value	Changing (%)* (increasing (+), decreasing (-))
TPPR(°C)		65	55.19	-15%
PPPR(bar)		-2	-1.95866	-2%
MFT_{icl4} (kg/hr.)		300	107.97	-64%
M_{FTEA} (kg/hr.)		10	3.93	-61%
1/(Polypropylene productivity (kg/hr.))		1.99×10^{-4}	1.42×10^{-4}	-41%
Productivity of Polypropylene (kg/hr.)		5021.33	7058.85	+41%
$\text{Changing}(\%)=\frac{(\text{Simulation value-Optimization value})}{\text{Simulation value}}\times100\%$				

The upper and lower bounds of these variables have been presented in Table 10. As mentioned in the sensitivity analysis section and figures, these variables affect PP productivity differently. Therefore, using these parameters as decision variables of the PP unit is necessary. Fig. 21 shows the optimal solutions obtained for the problem after performing 40 steps of population generation for the decision parameters listed in Table 13. In this figure, the optimal values of the productivity of polypropylene (PP) and reverse are drawn based on each other. As mentioned above, polypropylene productivity as the main objective optimization of integrated plant has a 41% increase by using the SCA optimization algorithm for integrated natural gas to polypropylene plant, and all 8 decision variables were changed (as seen in Table 13).

Suppose from an economic point of view, which is an essential aspect for production units, the increase in production due to the using optimal operating conditions is considered. In that case, the income increase in one year will equal 44.12 M$, which is a significant income. Fig. 22 represents the polypropylene global cost.

$$\text{Annual PP Productivity Development (Ton)}=\text{Polypropylene productivity}\left(\frac{kg}{h}\right)\times \text{Facor(1)}\left(\frac{h}{day}\right)\times \text{Facor(2)}\left(\frac{day}{yr}\right)\times \text{Facor(3)}\left(\frac{MT}{kg}\right) \quad (26)$$

$$\text{Facor(1)}\left(\frac{h}{day}\right)=24 \quad \text{Facor(2)}\left(\frac{day}{yr}\right)=330 \quad \text{Facor(3)}\left(\frac{MT}{kg}\right)=0.001 \quad (27)$$

$$\text{Annual PP Productivity Development (MT)}=(7058.85-5021.33)\times 24\times 330=2037.52\times 24\times 330=1637\left(\frac{MT}{yr}\right) \quad (28)$$

Raw annual income ($)=Polypropylene productivity (MT/y)×Cost of polypropylene ($/MT) (29)

Raw annual income ($)=16137 (MT/y)×2734 ($/MT)= 44.12 ((M $)/y) (30)

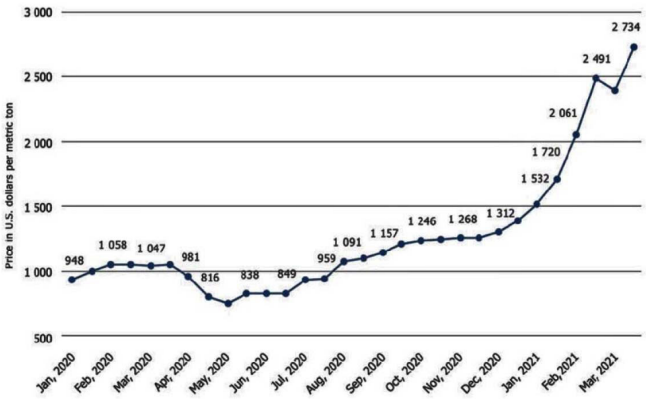

Fig. 22 Price of polypropylene from January 2020 to March 2021 [46].

Conclusions

The simulation of natural gas to polypropylene unit was done using the integration of Aspen HYSYS and Aspen Plus. The effective parameters to achieve the maximum propylene productivity as an optimization objective function in propylene and polypropylene units were determined by sensitivity analysis by changing the value of the effective parameter as optimization decision variables.

Some basic ones that affect the objective function were selected among these variables. The single objective optimization was carried out using the SCA algorithm, and the obtained optimal results are displayed in the table (Table 13) and figure (Fig. 22).

Decision variables included:

$T_{Ref.gas}$ (°C), T_{MeOH}(°C), R_{HC} (unit less), P_{MeOH} (kPa), T_{PPR}, P_{PPR}, M_{FTicl4}, MFTEA

These decision variables have different effects on the objective function. In this simulation, recycling unreacted hydrocarbons to the synthesis gas, methanol, and polypropylene production units increased PP productivity.

According to the sensitivity analysis, with the increase in the production temperature of the reformer gas, the ratio of H_2/CO gas decreases. Accordingly, the amount of propylene and polypropylene product production decreases.

Also, with the increase in the temperature of the methanol synthesis reactor, the conversion percentage of the methanol production reactor decreases. As a result, the amount of propylene and polypropylene produced decreases. By increasing the pressure of the methanol synthesis reactor, the conversion percentage of the methanol synthesis reactor increases, and as a result, the productivity of propylene and polypropylene increases. The ratio of returned hydrocarbon to the methanol synthesis reactor from 0.1 to almost 0.63 increases the produced product and remains almost constant. Using the results obtained from the SCA optimization algorithm, the temperature of the reformer gas at 875 °C, the temperature of the methanol synthesis reactor at 225.91 °C, the pressure of the methanol synthesis reactor at 140.81 bar, the return hydrocarbon ratio at 0.7 and the feed temperature entering the polypropylene reactor at 55.19 °C, mass flow of CAT stream 107.97 kg/h, and mass flow of COCAT stream 3.93 kg/h, the maximum productivity of polypropylene product is about 7058.85 kg/h (55906 Ton/y) obtained. The optimization results showed that the PP productivity increased by about 41% compared to the base state. Also, from the income point of view, this increase in productivity was calculated to be equivalent to an increase in income of 44.12 M$ per year.

Nomenclatures

Sinus-Cosine Algorithm: SCA
Natural Gas: NG
Methanol to Propylene: MTP
Propylene to Polypropylene: PTPP
Propane Dehydrogenation: PDH
Polypropylene: PP
Methanol to olefin: MTO
Melt Flow Index: MFI
Triethylaluminium: TEAL

Greek Letters

Reformer gas production Temperature: $T_{Ref.gas}$
Methanol production Temperature: T_{MeOH}
Inlet feed Temperature to PP production reactor: T_{PPR}
The pressure of the methanol synthesis reactor: P_{MeOH}
The ratio of hydrocarbon return flow rate to methanol synthesis reactor: R_{HC}
Temperature of the input feed to the polypropylene production reactor: T_{FtRPP}

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