Original Article: Optimization and Simulation of Process Unit in the Chemical Industry

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Citation P. Shirzadi*, **Optimization and Simulation of Process Unit in the Chemical Industry.** *J. Eng. Indu. Res.* 2022; 3(3):153-160.

https://doi.org/10.22034/JEIRES.2022.3.6

Article info:
Received: 07 December 2021
Accepted: 04 February 2022
Available Online: 04 February 2022
ID: JEIRES-2201-1065
Checked for Plagiarism: Yes
Peer Reviewers Approved by:
Dr. Amir Samimi
Editor who Approved Publication:
Professor Dr. Mohammad Haghighi

Keywords:
Simulation software; Chemical industry; Free optimization; Aspen Plus software

ABSTRACT

Simulation of process units to optimize them has long been considered in the chemical industry. Limited sources of energy supply and their increasing consumption in various industries have made optimization and subsequent energy integration important. There are many alternatives to designing a new process or optimizing an existing one, which can waste time and energy and increase costs. But with simulation software, the speed of estimating alternatives has increased. On the other hand, the optimization features in this type of software have caused the comparison of different processes to be made in the best possible way. This is because different alternatives should be compared and selected in optimal conditions. Aspen Plus software has process optimization features that the user can easily optimize the simulated unit by defining the objective function and existing constraints and free optimization variables. The user must first extract the objective and constraint function variables from flow Sheet 1 and define the objective function and constraints by combining these variables. Also, free optimization variables should be introduced from the available variables selected for optimization. In this research study, optimization was done to produce 6 MW power.

Introduction

Introduction of variables

1- Fuel cell operating temperature: Considering that most research have been conducted to reduce the operating temperature of the fuel cell (while maintaining high performance), we also assume the operating temperature of the fuel cell 1100 K and the performance of the whole system according to this the temperature is measured [1].

2- Flow density: Flow density is one of the most critical design variables on which the efficiency of the composite system is highly dependent. Decreasing the current density increases the

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efficiency of the system. However, if the current density decreases too much, then the level used in the cell will increase sharply, and as a result, the economic costs will increase. According to the operating temperature of the fuel cell, the selected range for optimization is in the range of 0.1-0.8 A/cm^2

3- Input fuel: Input fuel citizenship in terms of current density is as follows, assuming the production of net power of 6 MW. K is a constant value controlled by the logical operators of Aspen Plus [2-4].

(1) fNG (mot) = 1.0741 × io.o72 × k 0.05 < i ≤ 0.8 0.95 < k < 1.1

4- Boiler exhaust gas temperature: Due to the arrangement of converters, boiler exhaust gas temperature dramatically affects the economy of the problem. The temperature variation is between 200-500 degrees Celsius. This temperature limit is determined based on the type of converters.

5- Inlet pressure to the steam turbine: This pressure is adjusted so that while having the highest efficiency, the temperature of the inlet steam to the reboiler is in the superheated state and has a maximum distance of 20 °C from the saturation point. The reason is to prevent the formation of liquid during the transfer of water vapor to the reboiler [5].

6- Intermediate pressure of recovery cycle: The amount of this pressure depends on the economic conditions of the problem, the range of which is between 1000-4000 kP.

7- Generator temperature: This temperature dramatically affects the combined cycle's performance and absorption chiller cycle's performance and cost. According to the results, the appropriate range for this temperature is 125-150 °C, where the desired point is selected according to the optimal conditions [6].

8- Water consumption:

Optimizing water consumption in absorbers, condensers, and rectifiers plays an essential role in reducing fixed and operating costs. The price of water consumption is an essential factor in finding the optimal point. As the amount of water consumed increases, the level used in the converters decreases, and as a result, fixed costs decrease, but operating costs due to the price of consumed water increase. Therefore, it is necessary to determine the optimal point by balancing these two types of costs [7].

The variables to be optimized include flow density, boiler outlet temperature, steam turbine inlet pressure, mid-recovery cycle pressure, consumption temperature, and water consumption [8].

To optimize a process, it is necessary to make economic estimates because the economic conditions determine what kind of design is appropriate and optimal and whether the process is cost-effective. Of course, the point to be noted today is that environmental conditions significantly impact the structural and operational design of the process. This means that additional costs must be incurred to reduce the entry of pollutants into the environment. This additional cost can be done structurally or operationally on the process. However, the costs of a design still need to be calculated. The costs required to build a new process include fixed capital investment costs and the costs incurred from starting the process to the production stage (working capital investment) [9].

Fixed Capital Costs

These costs include the cost of purchasing and installing equipment. The purchase cost of each component is extracted according to the relationships in different sources, and the other costs are estimated based on the equipment purchased. These coefficients are obtained according to work done in combined cycle power plants and fuel cell power plants that run on natural gas. It should be noted that the cost of ammonia-water absorption chiller has been calculated separately based on the work of Carles *et al.* [10]. The cost of each piece of equipment is based on the year 2007 and in US dollars.

Heat exchangers [11]

(2) Air preheater1 $20 < A < 140\ m^2$ \$ = 5400 + 420A

(3) Air preheater2 $4 < A < 30\ m^2$ \$ = 293 × Aଢ.48

(4) Boiler $20 < A < 140\ m^2$ \$ = 1800 + 1200A

(5) Fuel preheater $4 < A < 30\ m^2$ \$ = 367 × Aଢ.48

To estimate the cost of converters used in absorption chillers, we use the following equation [29,30]:

(6) \$ = 268.42 + 561.6A

To calculate the level used in converters, we use the following equation:

(7) Q = U × A × LMTD

The overall heat transfer coefficient (U) is estimated according to the fluid passing through the transducer, the values of which are reported for each of the transducers in Table 1:

Table 1: Values of total heat transfer coefficient

Heat exchanger	**U(kW.m² K)**
Air preheater	**30-35 [2]**
Boiler	**40 [3]**
Fuel preheater	**30-35 [4]**
Condenser	**1100 [4]**
Evaporator	**1340 [5]**
Absorber	**910 [4]**
Reboiler	**1100 [2]**
Rectifier	**1000 [5]**
SHX	**990 [5]**
RHX	**1000 [۳]**

Pump

To calculate the price of pumps used in the process, we use the following equations [31]:

(8) V (m^3.s): volume flow rate m = 0.0544[log(V)]^2 + 0.5738 ×log(V) + 4.4

(9) P101-CW \$ = 0.664 × 10m

(10) P101-ABC, P101, 102-SC \$ = 1.4 × 10m

(11) P103-SC \$ = 3.6 × 10m

Engine [12]

(12) \$ = 1.91 × [exp(5.329 + 0.05048ln(hp)]

Compressor [13-15]

(13) Air compressor (1) \$ = 2910 × Wo.7ଢ

W (kW): work

(14) Fuel compressor \$ = 2040 × Wo.7ଢ

W (kW): work

(15) CGR \$ = 6.5 × (309.12 × V + 822.7)

(16) AGR \$ = 6.8 × (309.12 × V + 822.7

Steam turbine [16]

Mass solid oxide fuel cell [17]

(17) \$ = 1260 × W٠.8

(18) Cell cost: \$ =2

(19) Other cost (install cost, inverter cost …):

\$ =Ac Power(kw)

Combustion chamber and pre-reformer [18]

(20) Catalytic combustor $ =Ac Power (kw)

(21) Catalytic pre-reforming $ =Ac Power (kw)

Other fixed costs of the process are estimated according to the price of the purchased equipment according to different sources, which are as follows: [19]

P= Purchased equipment cost

Piping and installation: 0.35

Control and electrical: 0.2

Construction cost including: 0.1

Service facilities: 0.1

Civil structural: 0.15

Engineering and supervision: 0.25

Contingencies: 0.2

(22)

Land: $$\$ = \frac{2}{AC\ Power(kW)}$$

Working Capital

Which includes the total cost (raw materials, labor, and maintenance) to prepare the process for production, which is estimated based on the price of equipment purchased [20].

Working capital: 0.3

(23) Initial cost for catalyst:

$$\$ = \frac{2}{AC\ Power(kW)}$$

Total Capital Investment

The total set of fixed and operational costs equals the total investment made for a process up to the production stage. We assume that the money needed to invest is borrowed over several years at a fixed interest rate to convert this cost into an annual cost. According to the following formula, the total investment is converted into an annual cost compared to the costs incurred during the process. In this formula, n is the borrowing time, and i is the interest rate [16].

(24)

$$Annulized\ capital\ cost = Capital\ cost \times \frac{i\times(1+i)^n}{(1+i)^n-1}$$

Production cost

Production costs include costs to be incurred during the production process. The fuel required to enter the process, the cell surface to be replaced, the catalyst required, and the amount of water consumed are among the most essential costs. In this project, the degradation rate of solid oxide fuel cell is considered 0.5% every 1000 hours, and it is replaced every 5 years. By multiplying the appropriate coefficients, all production costs are expressed per year to be added to the annual investment cost [17].

Natural Gas cost (HHV): $$\$ = \frac{8}{MMBtu} = \frac{0.0273}{KWh}$$

Cooling water cost: $$\$ = \frac{0.05}{m^3}$$

Labor cost: 10% total Product cost

Other production cost: 10-15% total Product cost

It should be noted that the depreciation fee was not included in the calculations [18].

Objective function

To optimize a process, it is necessary to introduce a function and examine the effect of all the desired variables on it simultaneously. One of these functions is the sum of fixed costs (annually) and production costs:

(25) Total Annual Cost (TAC) = Fixed cost + Variable cost

The following function is also one of the options for optimizing the system:

(26) Economic potential (EP) = value of product - Fixed cost - Variable cost

Necessary process outputs include generated electricity and generated cooling. For pricing on generated cold, this cold can be converted into equivalent electricity, and then its value can be determined according to the price of electricity. The electricity price can be determined so that the set price can offset the fixed costs and current costs and, in fact, become EP=0. One of the parameters that determine the annual profit of the unit is the number of days that the unit works per year. In this project, it is assumed that this unit will operate in 90% of the days of the year and will have a lifespan of 20 years [19-21]. The interest rate is also assumed to be 10%. According to the above, the share of each cost in determining the price of electricity can be expressed as follows. Since prices (including fuel) change during the unit's life, the calculated electricity price is suitable for the first year of unit operation. To calculate the electricity price in later years, the inflation rate, depreciation cost, and global price changes must be calculated be considered. Fuel, etc., should also be considered in the calculations. Therefore, the price offered for electricity is based on the first year [22].

$$(27)\ C_{Capital\ cost}\left[\frac{S}{kWh}\right]=\frac{TCL\ (annual\ cost)\times CRF}{8766\times CF\times\ net\ Power(kW)}$$

$$(28)\ C_{Product\ cost}\left[\frac{S}{kWh}\right]=\frac{TPC\ (annual)}{8766\times CF\times net\ Power(kW)}$$

$$(29)\ COE=C_{Capital\ cost}+\ C_{Product\ cost}$$

COE = Cost Of Electricity

CRF = Capital Recovery factor (convert capital cost to annual cost)

CF = Capacity Factor (fraction of year that plant is in operation)

Consequently, COE can also be selected as the objective function, which due to its nature we try to minimize. Other functions for which the performance of the process can be measured is the amount of cost incurred to the production capacity by the process:

$$(30)\quad Cost\ per\ power=\frac{Total\ capital\ investment}{Net\ Power(kW)}$$

Finally, the combined system, including solid oxide fuel cell system, Rankin recovery cycle, and ammonia-water adsorption cycle, is optimized according to the COE objective function. It should be noted that the actual electricity price should be calculated based on the solid oxide fuel cell system and the Rankin recovery cycle. Because these are the two systems responsible for generating electricity and are responsible for an absorption cycle of cold generation [23-25].

Therefore, in the presented results, two types of electricity prices have been reported, one based on the complete combined cycle (ABC + SC + SOFC) and the other based on the combined cycle without absorption cycle (SC + SOFC) [26-28].

Variables

1- Current density (0.61 A/cm^2): 0.05≤i≤0.8

2- Boiler outlet temperature (300 ◦C): 250≤T≤500

3- Inlet pressure to the turbine (8000 kPa): 5000≤P≤8700

4- Medium recovery cycle pressure (2000 kPa): 1000≤P≤3000

5- Generator temperature (129 ◦C) 125≤T≤150

6- Adjusting the tap in the absorber (7 ◦C) (adjusting the water consumption) 3≤T≤8

Limitations

1- T_{122} < 750

2- T_{103}-cw≤40

3- T_{120}< 1050

It should be noted that the efficiency of the DC-AC converter is 0.97 and other parameters are in accordance with previous chapters [29]. Before optimizing the values of each of the introduced economic parameters, the electrical efficiency, heat, and cold produced are summarized in Table 2:

Table 2: Pre-optimal values of economic parameters

Value	Unit	Parameters
TCI(FC+ST)	1000 $	957.2

TCI(ABC)	1000 $	179.7
TPC	1000 $.year	296
COE(FC+ST)	$/kWh	0.0923
COE(FC+ST+ABC)	$/kWh	0.0998
CPP(FC+ST)	$/kW	1915
CPP(FC+ST+ABC)	$/kW	2110
Elec. Eff.(LHV)	%	58.5
Power production	kW	500
Heat production	kW	38.67
Refrigeration duty	kW	115.3

Results

Aspen Plus software uses various optimization methods, including:

1- BOX method 2
2- SQP method
3- Fletcher-Reeves method
4- Quasi-Newton method
5- Mixed method (combination of BOX method and SQP method)

According to the problem conditions and the number of variables and constraints, we use method 2 for optimization. This method uses the Powell algorithm for optimization and is suitable as long as it has an excellent initial guess and few optimization variables [30]. This method can be used for optimization with equal and unequal constraints. Performing the optimization by Aspen Plus software, the values of each variable after optimization are reported in Table 3. Also, the desired economic parameters after optimization are reported in Table 4.

Table 3: Values of variables after optimization

Parameters	Unit	Value
i	A/cm^2	0.45
T123	°C	439
P101-SC	KPa	8700
P102-SC	KPa	1820
T112-ABC	°C	137
TAP	°C	6.1

Table 4: Values of economic parameters after optimization

Parameters	Value	Unit
TCI(FC+ST)	1000 $	902
TCI(ABC)	1000 $	136.4
TPC	1000 $. year	280.4
COE(FC+ST)	$/kWh	0.0893
COE(FC+ST+ABC)	$/kWh	0.0946
CPP(FC+ST)	$/kW	1805
CPP(FC+ST+ABC)	$/kW	1945
Elec. Eff. (LHV)	%	62.8
Power production	kW	6000
Heat production	kW	430.99
Refrigeration duty	kW	900.11

Figure 1 reveals the changes in electricity prices in terms of current density. However, the price of electricity in this figure is based on the solid oxide fuel cell system and Rankin recovery cycle, and the absorption cycle is not included in the calculations. According to this figure, the minimum price of electricity occurs at a current density of 0.44. However, the results obtained in Table 15 are based on the complete combined cycle. The electricity price of the whole cycle is introduced as an objective function, resulting in a minimum electricity price at a current density of 0.45.

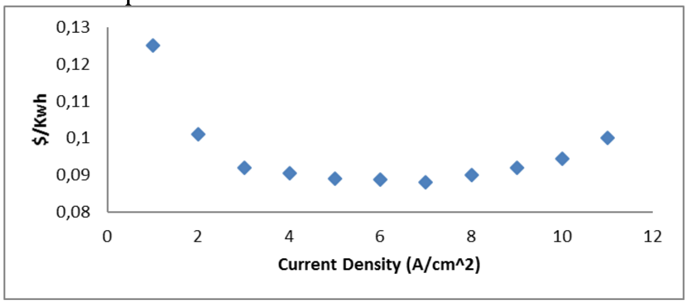

Figure 1: Electricity Price Changes (SOFC + SC) in terms of current density

As can be seen from the figure, the minimum investment cost occurs at a current density of 0.53, while the minimum price of electricity occurs at a current density of 0.44. This is because in calculating the price of electricity, both investment costs and production costs are taken into account. Table 5 compares the various parameters of the hybrid system before and after optimization.

Table 5: Comparison of hybrid system parameters before and after optimization

Parameter	Before Optimization	After Optimization
Voltage (V)	0.72	0.784
Current Density (cm^2)	0.61	0.395
DC Power (KW)	6010	6100
Net Power (KW)	6000	6100
Fuel (kg/h)	1225	1112
ST Power (KW)	725.5	510.98
Total Power Consumption (KW)	567	437.5
Total eff (HHV)	0.71	0.722
Elec. Eff (HHV)	0.45	0.48
Net eff (HHV)	0.65	0.67
Cell Area (m^2)	1150	1275
Heat exchanger area (m^2)	129.8	115.9
COP	0.629	0.642

Conclusion

Therefore, since the efficiency of the fuel cell increases with decreasing current density, the input fuel to the system decreases. As a result, the minimum price of electricity in the current density is lower than the minimum investment cost. Consequently, it can be decided to reduce the surface area used in the fuel cell mass from 0.395 to 0.6 square meters by increasing the current density from 165 to 115. The advantage of this work is that while significantly reducing the area used in the fuel cell mass, the increase in electricity prices and investment costs is very low. Its only drawback is the reduction of the electrical efficiency of the hybrid system.

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