

Development and Optimization of an Integrated Process Configuration for IGCC Power Generation Technology with a Fischer-Tropsch Fuels from Coal and Biomass

Malek Shariati Niassar

Renewable Energies and Environmental Department, Niroo Research Institute, Tehran, Iran

Received: 2018-09-01

Revised: 2018-10-20

Accepted: 2018-11-01

Abstract: The conversion of coal into high-quality fuels is carried out through gasification, syngas production and the process of Fischer-Tropsch. Additionally, produced syngas derived from coal gasification only can generate power and heat in a combined cycle power plant. In order to combine these two methods together in an integrated process at the same time, it is necessary to use part of the produced gas for the production of heat and power, and the other part for the production of liquid fuel. As a result, this new and integrated process will consist of three major parts: "coal gasification", "power and heat generation" and "production of liquid fuel". The purpose of this study is by consideration of an integrated gasification combined cycle (IGCC) plant with input feed of coal, an integrated system of "Combined heat and power as well as liquid fuel of Fischer-Tropsch", called in this research CHPF is designed, and the optimum amounts of production of the power, heat and liquid fuel are provided at a certain scale of the feedstock. Thus, the various parts of this integrated process is designed conceptually, and simulated and integrated with Aspen software; then an objective function is defined to maximize the revenue from the sale of process products (power and liquid fuels). To ensure the accuracy of the results, the sensitivity analysis tool is used; and the simulation and design results are compared with an experimental work, indicating that the difference in results is about 4%.

keywords: Gasification of coal, Cogeneration, production of liquid fuels, Fischer-Tropsch, sensitivity analysis

1. Introduction

The conversion of coal into high-quality fuels is carried out through gasification, syngas production and the process of Fischer-Tropsch which is called liquefaction of coal. Another usage of coal gasification is to employ the produced syngas derived from coal gasification to generate power and heat in a combined cycle power plant. The gasification process has been commercially used for more than a century to produce fuel and chemicals. The conversion of coal into higher quality fuels is carried out through gasification and syngas production.

Coal produces have the highest amount of CO₂ per unit produced heat and electricity among all fuels, consequently anxieties about global warming have cause much work on operative CO₂ recovery from power generations. Even though many methods have

proposed for capturing of CO₂ in the power generation sectors, they naturally result in considerably lowering the plant energy efficiency and surging in the cost of electricity owing to the high energy consumption. IGCC which stands for integrated gasification combined cycles, can be used because of the high efficiency of combined cycles for power generation, most conveniently need gaseous fuel, where the coal is first altered into syngas in a gasifier, which is then used to fuel the gas turbine in the combined cycle (Chen et al., 2015).

Biomass is considered as a low carbon source for various energy or chemical options (Daioglou et al., 2015). Biomass during its growth is the lone source which can store solar energy in the chemical bond. The stored energy is able to be applied for thermochemical conversion of biomass.

* Corresponding Author.

Authors' Email Address: M. Shariati Niassar (malekshariati@gmail.com)

ISSN (Online): 2345-4172, ISSN (Print): 2322-3251

© 2018 University of Isfahan. All rights reserved

Gasification, converting biomass to flammable gases, is considered as one of the capable thermochemical conversion technologies (Asadullah, 2014). Current techniques and new development in gasification and pyrolysis techniques for the conversion of cellulosic biomass into a viable source of energy have been scrutinized. Biomass gasification for producing syngas, bio-oil, co-firing of coal and biomass as well as using gasification and co-pyrolysis at the same time, synthesis of pyrolysis and gasification to process pyrolysis yields to syngas using gasification and liquefaction and converting to fuels like, methanol, ethanol, and Fisher-Tropsch oil using modified catalysis (Digman et al., 2009). The status and prospects of biomass value chains for heat, power, fuels, and materials have been investigated for optimizing and developing biomass application in a sustainable way. Additionally, evaluation of current and long-term leveled production costs and avoided emissions as well as greenhouse gas abatement costs have been carried out (Gerssen-Gondelach et al., 2014). A clean power plant is constructed based on the steam co-gasification of biomass and coal in a quaternary fluidized bed gasifier. The solid oxide fuel cell and the steam turbine are united to generate power. The chemical looping with oxygen uncoupling technology is employed for supplying oxygen, while the calcium looping and mineral carbonation are used for CO₂ capture and sequestration (Yan & He, 2017). Solid fuel decarbonisation by capturing CO₂ stemmed from thermochemical conversion of solid fuel using gasification. Assessment is concentrated on power generation technology using syngas produced by solid fuel gasification, called integrated gasification combined cycle. A mixture of biomass and coal is employed to produce around 400 MW electricity at the same time with capturing 90% of carbon in feedstock (Cormos et al., 2009).

hybrid energy systems are employed for poly-generation targets (Ghorbani, Shirmohammadi, & Mehrpooya, 2018; Ghorbani, Shirmohammadi, Mehrpooya, & Mafi, 2018). Exergy and energy analyses have been employed for evaluating of various processes and the above-mentioned systems. (Ghazizadeh et al., 2018; Hamed et al., 2015; Sheikhi et al., 2014). Examining the energetic performances of biomass Organic Rankine Cycles for domestic micro-scale CHP generation has been carried out. A parametric

analysis also has been done for diverse ORC configurations (Algieri & Morrone, 2014). Energy, exergy and exergoeconomic analyses are employed to evaluate a gas turbine cycle with fog cooling and steam injection, integrated by biomass gasification. The thermodynamic analyses show that surging in the compressor pressure ratio and the gas turbine inlet temperature can increase the energy and exergy efficiencies (Athari et al., 2015). Exergy analysis is also employed for evaluation of biogas production from a municipal solid waste landfill (Salomón et al., 2013). Woody biomass by gasification has been employed for producing hydrocarbon liquid fuel with daily production of the biomass-to-liquid equal to 7.8 L of hydrocarbon liquid from 48kg of woody biomass equivalent to 0.05 barrels (Hanaoka et al., 2010). In many researches, the importance of operational parameters optimization has been investigated (Ghorbani, Shirmohammadi, Mehrpooya, & Hamed, 2018; Shirmohammadi et al., 2015). Operation and performance of a polygeneration solar-hybrid CTL incorporating solar resource has been investigated, and energetic and environmental performance of process is compared for validation (Kaniyal et al., 2013). Energy optimization in a GTL unit with a capacity of 10, 000 BPD are studied at different levels of the process using optimizer software (Amidpour et al., 2009). A mixed integer linear programming is employed to optimize multi-biomass and natural gas supply chain design with concentration on temporal distribution of biomass supply, processing, storage, transport and energy conversion to meet the required heat of residential end users (Pantaleo et al., 2014a). A biomass CCHP system containing a biomass gasifier has been analyzed using energy and exergy analyses (Wang et al., 2015). A solid oxide fuel cell and an integrated gasification with a steam cycle as well as gas turbine consuming heat recovery of the gas turbine has been analyzed by energy and exergy analyses (El-Emam et al., 2012). Enhancing exergetic efficiency of a cryogenic ASU in an IGCC has been investigated. Techno-economic and sensitivity analyses are also carried out for the aforementioned system (Pantaleo et al., 2014b). Energy efficiency analysis has been done for a solar aided biomass gasification for producing pure hydrogen (Salemme et al., 2014). CO₂ avoided emissions and economic

analyses of WWTP biogas recovery and its usage in a power generation in Brazil have been investigated (dos Santos et al., 2016). Energy and environmental analyses are employed for evaluation of a small-scale biomass gasification CHP (Xydis et al., 2013). Thermodynamic, economic and environmental evaluation have been employed for analyzing gasification process application in electrical energy-freshwater generation from heavy fuel (Meratizaman et al., 2015). Investigation of the influence of operating conditions on performance of a SOFC by integrated gasifier has been carried out. The main aim of the study is to examine the integration of a biomass gasifier process with the SOFC in a systematic and wide procedure (Campitelli et al., 2013).

A solar hybridized dual fluidized bed gasification process is projected with char separation for producing liquid fuels of Fischer-Tropsch from solid biomass with or without coal. It is concluded that the specific FT liquids output per unit feedstock of the system declines with an surge in the biomass fraction because of the higher content of light hydrocarbons content in the syngas produced with the studied biomass gasification (Guo et al., 2017). Electrically heated gasifier with sand particles fluidized bed is employed for the coal slurries gasification (Svoboda et al., 2012). An alternative technology, i.e. simulated moving bed technology, to conventional coal gasification is debated for enhancing the performances of the current processes (Sudiro et al., 2010). An integrated system combining biomass gasification, chemical looping combustion, solid oxide fuel cell system and a steam power cycle has been developed. Sensitivity analysis is also carried out for main parameters to analyze the performance of the integrated system and investigation of the optimal operating condition (Aghaie et al., 2016). Another solid oxide fuel cell system integrated with hybrid biomass gasification as well as enhanced CHP plant has been examined using advanced non-incineration conversion methods for generating power (Mustafa et al., 2017).

Fuels particularly diesel attained from the syngas conversion by Fischer-Tropsch synthesis have high quality. It also can contribute considerably to protection of environment and surging in the amount of energy efficiency. In recent years, Fischer-Tropsch synthesis technology has been developed for constructing of large-scale complexes to reach economical aims in several

cases (Y.-W. Li, 2004). Development of gas cleaning technology has been carried out for two integrated biomass gasification and Fischer-Tropsch (FT) synthesis systems. Results show that there are not any impurities in biomass-derived syngas involving a completely diverse gas cleaning approach in comparison with coal or natural gas based syngas production for FT synthesis (Boerrigter et al., 2004). Aspen Plus®-based process model has been employed to explore the influence of H₂/CO ratio in syngas from a biomass gasifier, efficiency of CO₂ removal, addition of a reformer in a recycle mode, the type of a Fischer-Tropsch catalyst, and co-feeding of natural gas and biomass on efficiency and prices for the producing liquid fuels from the biomass-derived syngas (Rafati et al., 2017). A process for producing waxes of Fischer-Tropsch using biogas has been developed. It is concluded that in one process step, the specific composition of biogas permits the production of syngas appropriate for Fischer-Tropsch synthesis (Herz et al., 2017).

The main objective of this paper is that by using conceptual design and utilizing software tools, in the CHP system on a specific scale of coal input feedstock, part of the syngas produced from the gasification process is allocated to the power generation and the other part is assigned to sector for the production of liquid fuels, so that the most revenue from the products is derived from the specific price of a given feed. To this end, an objective function is assumed to be that the amount of each product and its price are considered as the main factors and the percentage of syngas to each sector with the aim of achieving the highest revenue from the sale of power and liquid fuel production is determined.

2. Conceptual Process Design

Gasification is a way to convert low-value feedstock (coal, biomass and oil waste) into electricity, steam and also hydrogen used to produce cleaner fuels in transportation industry. The main parameter required for the feed used in the coal and biomass gasification unit is that the feed contains both hydrogen and carbon. For simulating of integrated combined heat and power, and liquid fuels using gasification of feedstock like coal and biomass, the following operation units are developed. These units are consists of:

- Sizing unit of the coal
- Gasification unit
- Air Separation Unit (ASU)
- Gas cleaning unit
- Water-gas shift
- Combined cycle power generation

Fig. 1 shows schematic of the process of integrated gasification system and CCHP and liquid fuels of Fischer-Tropsch. In this figure, the main units and connection of process streams and utilities are presented. The main steps are presented as follows:

- Coal in sizing unit is mixed with water to achieve the appropriate size for gasification process by crushing and screening operations. Lastly, the slurry of coal for the production of synthesis gas is entered into the gasification section.
- Gasification process requires oxygen, and required oxygen is supplied from the air separation unit (ASU). In this unit, air after initial treatment turns into nitrogen and oxygen. Required oxygen purity of

process must be suitable for gasification process. In this study, oxygen with molar purity of 95% is produced from ASU.

- Coal-Water slurry with oxygen with purity of 95% are mixed in gasification unit and turns into synthesis gas with low heating value.

• Corrosive components such as sulfides, nitrides and dusts are separated from the production synthesis gas in cleaning unit. Rehabilitation of rich H₂S from acid gas removal system to produce sulfur will be sent to the Claus unit.

• The WGS unit is intended to adjust the H₂/CO ratio required for the Fischer-Tropsch process. In this unit, the WGS reactor along with a cooling system are used to convert CO to CO₂.

• The produced syngas is divided into two parts. A part of it is enter into the FT unit and converted into fuel, and another part is entered into the combined power cycle unit for generating electricity and power.

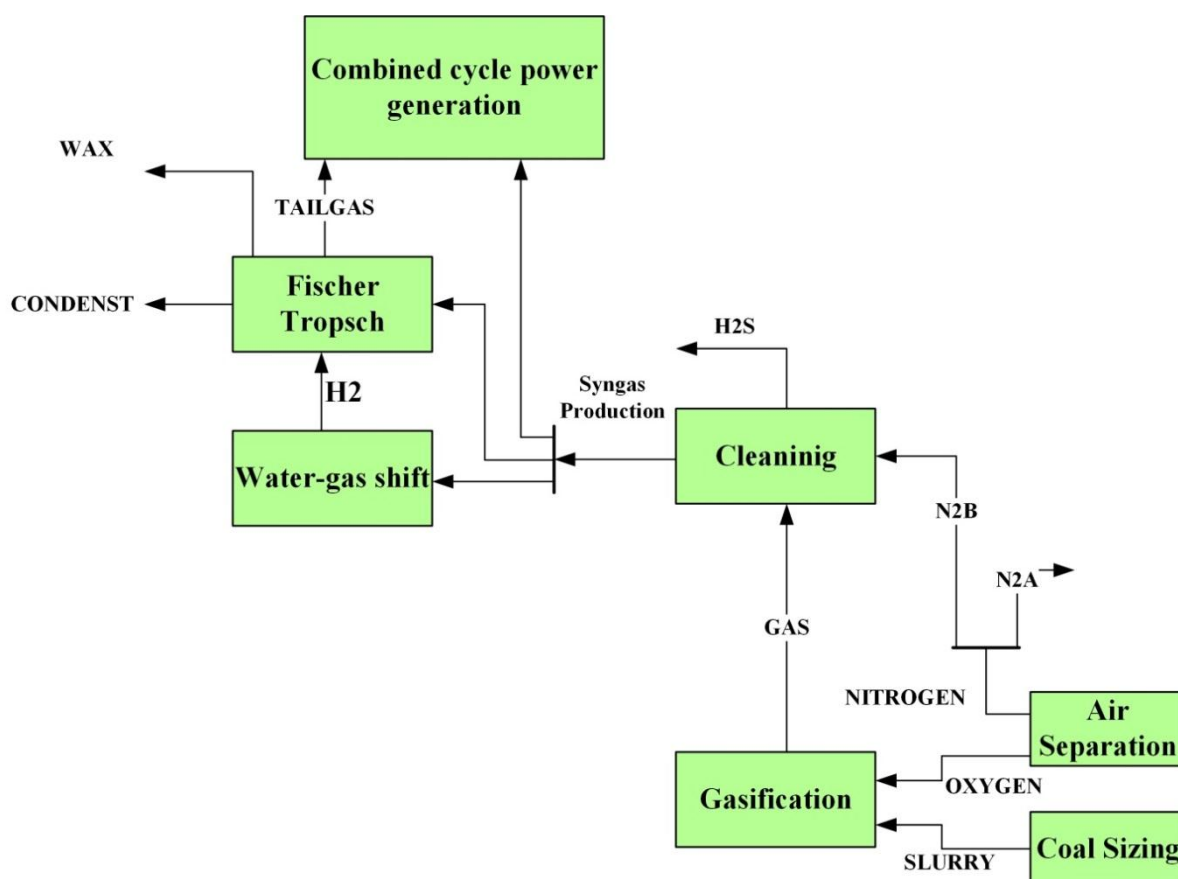


Figure 1. The overall scheme of the integrated system including gasification, cogeneration and production liquid fuel

2.1. Simulation Methodology

Preciado et al. (Preciado et al., 2012) produced syngas using Aspen Hysys software and coal gasification with input feedstock method. They used the air separation unit to supply the oxygen required by the gasifier. In this research, for the simulation, the reactions of this section are divided into three groups of coke decomposition reactions, coal feedstock, and gasification and hydrolysis of carbonyl sulfide. The NANMET energy technology center used Aspen software and simulated a number of Integrated Gas Combined Cycles (IGCCs); in these studies, a variety of gasifier technology such as Shell, Texaco, KRW and BGL (British Gas Lurgi Gasifier) were studied and models developed with Aspen software were compared with industrial data. In all cases, there is a good agreement between industrial data and software models. Based on the experience gained during simulation of the IGCC factories, the development of models for power generation plants was also achieved (Hlavacek et al., 1994; L Zheng & Furimsky, 1999). A third example from the use of Aspen software to simulate the gasification process is sugar cane bagasse presented by Mavukwana and his colleagues (Mavukwana et al., 2013), which compared their results with experimental results, and a good agreement between data and model results was obtained. In the fourth instance, Ramzan et al. developed a stable model for the study of gasification of municipal solid waste, poultry waste and food with the help of the Aspen Plus software. They investigated the effect of stoichiometric ratio of air to feedstock, temperature of gasifier, and moisture content of feedstock on performance of gasifier. Also, Sharmina Begum and his associates (Begum et al., 2014) provided a model using Aspen software for gasification of municipal solid waste. The results of the model show that there is good compatibility with the experimental data and the error of percent combined of output syngas from the gasifier with the experimental data is about 4%.

In this article, Aspen Plus was chosen as a computer software for process modeling as discussed in the selection of appropriate platform selection. In this paper, all of the above-mentioned process units were developed in the software environment and integrated together so that one can study the effect of a change in the operating conditions of a unit on other process units. According to this issue that the gasification unit is the core of the process model, thus the accuracy of modeling and

simulation of this unit is essential. The simulation of the gasification process is based on the balance of mass, energy, and chemical balance, and Aspen software provides a broad ability to simulate the process. The software includes several databases including physical, chemical, and thermodynamic properties for a wide range of chemical components along with the required thermodynamic model to simulate accurately chemical systems. The developed model in the software environment was blocked and a sequential solution method was used to solve the model equations. In developing each block model, the following are considered:

- Specify the process flow class
- Choosing the appropriate thermodynamic equation
- Identification of chemical components and determining the type of Conventional and Non-Conventional
- Defining of Process flow sheet (using operational blocks and connecting mass and energy flows)
- Identification of feed flows (flow rate, component composition and operating conditions)
- Identification of operational blocks (operating conditions, chemical reactions, etc.)

2.2. Definition of Chemical Reactions

The chemical reactions of the existing process are complex, and in this model, simpler methods have been used that have more experimental basis. These reactions are modeled by the RStoic, REquil and RGibbs models. Types of reactor models are:

RStoic, RYield, REquil, RGibbs, RPlug, RCSTR and RBatch.

- ✓ The RBatch, RCSTR and RPlug reactors are extreme models for Batch, CSTR, and Plug-in reactors.
- ✓ The RStoic model is used for samples that are stoichiometric, but reaction kinetics are either passive or negligible.
- ✓ If the kinetics and stoichiometry of the reaction are both passive, RYield should be used.
- ✓ For a single-phase chemical equilibrium or fuzzy chemical equilibrium, REQUIL or RGibbs reactor model calculations are performed.
- ✓ The REquil model runs on the basis of simultaneous computing of chemical stoichiometric or fuzzy equilibrium, while RGibbs reactors operate on the basis of minimizing Gibbs free energy.

The reactions in each reactor with their specifications are given below.

2.2.1. Coal Gasification Reactions

The reactions in this section are divided into three groups of reactions decomposition of coke, biomass feedstock, gasification and hydrolysis of carbonyl sulfide.

In the modeling of this section, decomposition reactions are considered in accordance with the above table and the RStoic model is used for this purpose. The stoichiometric coefficients of these reactions are the function of feedstock characteristics and determine the yields of the products. In coal gasification, if the purpose of the design is to design the reactor alone and to carefully examine the behavior of its components, kinetic models are used, but when it is used in conjunction with other units and in the form of flow sheet, the Gibbs model is used. In similar cases, the same model has been used and shown that the results with the experimental reactor have small differences and acceptable (X. Li et al., 2001). In this research, the Gibbs free energy minimization model is used, and the corresponding model is used in the RGibbs software environment. For hydrolysis of

carbonyl sulfide, the following reaction is performed in the RStoic model.

2.2.2. Power Generation Reactions

Reactions in this section are consist of combustion reactions of H₂, CO and CH₄ to hexane. Due to the high temperature of the reactions, the percent conversion is assumed to be 100%. All reactions in the power generation sector are modeled with the RStoic model. Since the input feed to the power plant includes syngas and Tail Gas of the Fischer-Tropsch production unit is defined, hence the two categories of syngas combustion and associated gas combustion are defined in this unit.

2.2.3. Water-Gas Shift (WGS) Reaction

In this section, water-gas shift (WGS) reaction is carried out, and CO is converted to CO₂ and H₂. In this section, adjusting of the hydrogen ratio to carbon monoxide is occurred. The water-gas shift (WGS) reaction is considered equilibrium, and is done using the REquil model in the software.

Table 1. Reactions Decomposition of Solid Feedstock

Rxn No.	Specification type	Stoichiometry	Fraction	Base Component
1	Frac. Conversion	COAL $\longrightarrow$ H ₂ O + O ₂ + N ₂ + C(Solid) + COALASH + S.S(Solid) + CL ₂ + H ₂	0.95	COAL
1	Frac. Conversion	BIOMASS $\longrightarrow$ H ₂ + O ₂ + N ₂ + C(Solid) + COALASH + S.S(Solid) + CL ₂ + H ₂	1	BIOMASS

Table 2. Syngas combustion reactions

Rxn No.	Specification type	Stoichiometry	Fraction	Base Component
1	Frac. Conversion	CO + 0.5 O ₂ $\longleftrightarrow$ CO ₂	1	CO
1	Frac. Conversion	H ₂ + 0.5 O ₂ $\longleftrightarrow$ H ₂ O	1	H ₂

Table 3. Reactions of associated gas combustion

Rxn No.	Specification type	Stoichiometry	Fraction	Base Component
1	CONVERSION	CH ₄ + 2 O ₂ $\rightarrow$ CO ₂ + 2 H ₂ O	1	CH ₄
2	CONVERSION	C ₂ H ₆ + 3.5 O ₂ $\rightarrow$ 2 CO ₂ + 3 H ₂ O	1	C ₂ H ₆
3	CONVERSION	C ₃ H ₈ + 5 O ₂ $\rightarrow$ 3 CO ₂ + 4 H ₂ O	1	C ₃ H ₈
4	CONVERSION	C ₄ H ₁₀ + 6.5 O ₂ $\rightarrow$ 4 CO ₂ + 5 H ₂ O	1	C ₄ H ₁₀
5	CONVERSION	C ₅ H ₁₂ + 8 O ₂ $\rightarrow$ 5 CO ₂ + 6 H ₂ O	1	C ₅ H ₁₂
6	CONVERSION	C ₆ H ₁₄ + 9.5 O ₂ $\rightarrow$ 6 CO ₂ + 7 H ₂ O	1	C ₆ H ₁₄
7	CONVERSION	CO + .5 O ₂ $\rightarrow$ CO ₂	1	CO
8	CONVERSION	H ₂ + .5 O ₂ $\rightarrow$ H ₂ O	1	H ₂

Table 4. Water-gas shift reactions

Rxn No.	Specification type	Stoichiometry
1	Temp. approach	Co + H ₂ O $\longleftrightarrow$ CO ₂ + H ₂

2.2.4. Fischer-Tropsch Reactions

This section includes reactions network of syngas conversion to a chain of hydrocarbons, which is subject to operating conditions and catalyst specifications. In the following table, the network of presented reactions is developed to simulate the Fischer-Tropsch unit, and the FT reactor model is developed with the reactions as well as help of the RStoic model of the Aspen software.

2.2.5. Definition of the Feedstock

Realistic methods are typically used to identify and analyze charcoal. These methods provide useful tools compared to methods for defining them in the form of pure chemical components for users. Two types of analyzes are used to define the coal (Higman & Van der Burgt, 2011), including Proximate analysis and Ultimate analysis. In addition to analysis of reference 38, the amount of sulfur in the coal is between 0.5 and 6% by weight, mainly in three forms of iron sulfide, inorganic sulfates and sulfur in existing mineral compounds. The

nitrogen existing in coal is in the range of 0.5 to 2.5% by weight, and only part of the nitrogen in coal in the gasification process is converted to ammonia and HCN, and the rest is converted into elemental nitrogen. Therefore, the presence of nitrogen in the gaseous product obtained from coal during the gasification process is one of the important reasons not to use high purity oxygen for the gasification process, even for the production of gas or hydrogen.

2.3. Simulation of System Process Units

2.3.1. Simulation of Coal Sizing Unit

The aim of this unit is to reduce the size of coal to achieve the appropriate size for gasification process. Therefore, in this unit crushing and screening operations of coal feedstock is carried out, and the slurry of coal for the production of synthesis gas is entered into the gasification section. Fig. 2 shows the overall schematic of the process.

Table 5. Fischer-Tropsch reactions

Rxn No.	Specification type	Stoichiometry
1	CONVERSION	$3 \text{ H}_2 + \text{CO} \rightarrow \text{CH}_4 + \text{H}_2\text{O}$
2	CONVERSION	$5 \text{ H}_2 + 2 \text{ CO} \rightarrow \text{C}_2\text{H}_6 + 2 \text{ H}_2\text{O}$
3	CONVERSION	$7 \text{ H}_2 + 3 \text{ CO} \rightarrow \text{C}_3\text{H}_8 + 3 \text{ H}_2\text{O}$
4	CONVERSION	$9 \text{ H}_2 + 4 \text{ CO} \rightarrow \text{C}_4\text{H}_{10} + 4 \text{ H}_2\text{O}$
5	CONVERSION	$11 \text{ H}_2 + 5 \text{ CO} \rightarrow \text{C}_5\text{H}_{12} + 5 \text{ H}_2\text{O}$
6	CONVERSION	$13 \text{ H}_2 + 6 \text{ CO} \rightarrow \text{C}_6\text{H}_{14} + 6 \text{ H}_2\text{O}$
7	CONVERSION	$15 \text{ H}_2 + 7 \text{ CO} \rightarrow \text{C}_7\text{H}_{16} + 7 \text{ H}_2\text{O}$
8	CONVERSION	$17 \text{ H}_2 + 8 \text{ CO} \rightarrow \text{C}_8\text{H}_{18} + 8 \text{ H}_2\text{O}$
9	CONVERSION	$19 \text{ H}_2 + 9 \text{ CO} \rightarrow \text{C}_9\text{H}_{20} + 9 \text{ H}_2\text{O}$
10	CONVERSION	$21 \text{ H}_2 + 10 \text{ CO} \rightarrow \text{C}_{10}\text{H}_{22} + 10 \text{ H}_2\text{O}$
11	CONVERSION	$23 \text{ H}_2 + 11 \text{ CO} \rightarrow \text{C}_{11}\text{H}_{24} + 11 \text{ H}_2\text{O}$
12	CONVERSION	$25 \text{ H}_2 + 12 \text{ CO} \rightarrow \text{C}_{12}\text{H}_{26} + 12 \text{ H}_2\text{O}$
13	CONVERSION	$27 \text{ H}_2 + 13 \text{ CO} \rightarrow \text{C}_{13}\text{H}_{28} + 13 \text{ H}_2\text{O}$
14	CONVERSION	$29 \text{ H}_2 + 14 \text{ CO} \rightarrow \text{C}_{14}\text{H}_{30} + 14 \text{ H}_2\text{O}$
15	CONVERSION	$31 \text{ H}_2 + 15 \text{ CO} \rightarrow \text{C}_{15}\text{H}_{32} + 15 \text{ H}_2\text{O}$
16	CONVERSION	$33 \text{ H}_2 + 16 \text{ CO} \rightarrow \text{C}_{16}\text{H}_{34} + 16 \text{ H}_2\text{O}$
17	CONVERSION	$35 \text{ H}_2 + 17 \text{ CO} \rightarrow \text{C}_{17}\text{H}_{36} + 17 \text{ H}_2\text{O}$
18	CONVERSION	$37 \text{ H}_2 + 18 \text{ CO} \rightarrow \text{C}_{18}\text{H}_{38} + 18 \text{ H}_2\text{O}$
19	CONVERSION	$39 \text{ H}_2 + 19 \text{ CO} \rightarrow \text{C}_{19}\text{H}_{40} + 19 \text{ H}_2\text{O}$
20	CONVERSION	$41 \text{ H}_2 + 20 \text{ CO} \rightarrow \text{C}_{20}\text{H}_{42} + 20 \text{ H}_2\text{O}$
21	CONVERSION	$43 \text{ H}_2 + 21 \text{ CO} \rightarrow \text{C}_{21}\text{H}_{44} + 21 \text{ H}_2\text{O}$
22	CONVERSION	$45 \text{ H}_2 + 22 \text{ CO} \rightarrow \text{C}_{22}\text{H}_{46} + 22 \text{ H}_2\text{O}$
23	CONVERSION	$47 \text{ H}_2 + 23 \text{ CO} \rightarrow \text{C}_{23}\text{H}_{48} + 23 \text{ H}_2\text{O}$
24	CONVERSION	$49 \text{ H}_2 + 24 \text{ CO} \rightarrow \text{C}_{24}\text{H}_{50} + 24 \text{ H}_2\text{O}$
25	CONVERSION	$51 \text{ H}_2 + 25 \text{ CO} \rightarrow \text{C}_{25}\text{H}_{52} + 25 \text{ H}_2\text{O}$
26	CONVERSION	$53 \text{ H}_2 + 26 \text{ CO} \rightarrow \text{C}_{26}\text{H}_{54} + 26 \text{ H}_2\text{O}$
27	CONVERSION	$55 \text{ H}_2 + 27 \text{ CO} \rightarrow \text{C}_{27}\text{H}_{56} + 27 \text{ H}_2\text{O}$
28	CONVERSION	$57 \text{ H}_2 + 28 \text{ CO} \rightarrow \text{C}_{28}\text{H}_{58} + 28 \text{ H}_2\text{O}$
29	CONVERSION	$59 \text{ H}_2 + 29 \text{ CO} \rightarrow \text{C}_{29}\text{H}_{60} + 29 \text{ H}_2\text{O}$
30	CONVERSION	$61 \text{ H}_2 + 30 \text{ CO} \rightarrow \text{C}_{30}\text{H}_{62} + 30 \text{ H}_2\text{O}$
31	CONVERSION	$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$

In this section, two Bitumous and Biomass feedstock have been entered to the process. The main feedstock is coal or Bitumous, but biomass feedstock can also be defined in the process so that coal feedstock can be switched by biomass feedstock. The flow of coal (with a flow rate of 126 tons per hour) is combined with water (with a flow rate of 53 tons per hour) and it then is entered into two crushing units of Bmill 1 and Bmill 2, and after screening by Screen, the particles with optimum size are sent to the gasification unit, and the coarser particles are returned to the beginning of the process. The power required

for grinding and crushing of the coal flow is provided by the power generation unit.

2.3.2. Simulation of Coal Gasification Unit

In this unit, gasification of feedstock is done. The gasification process involves a number of steps: drying, decomposition, gasification and combustion. The overall diagram of this unit is shown in Fig. 3. As it was mentioned in section related to feedstock, gasification feedstock should be defined as Non-conventional using Proximate and Ultimate analyses.

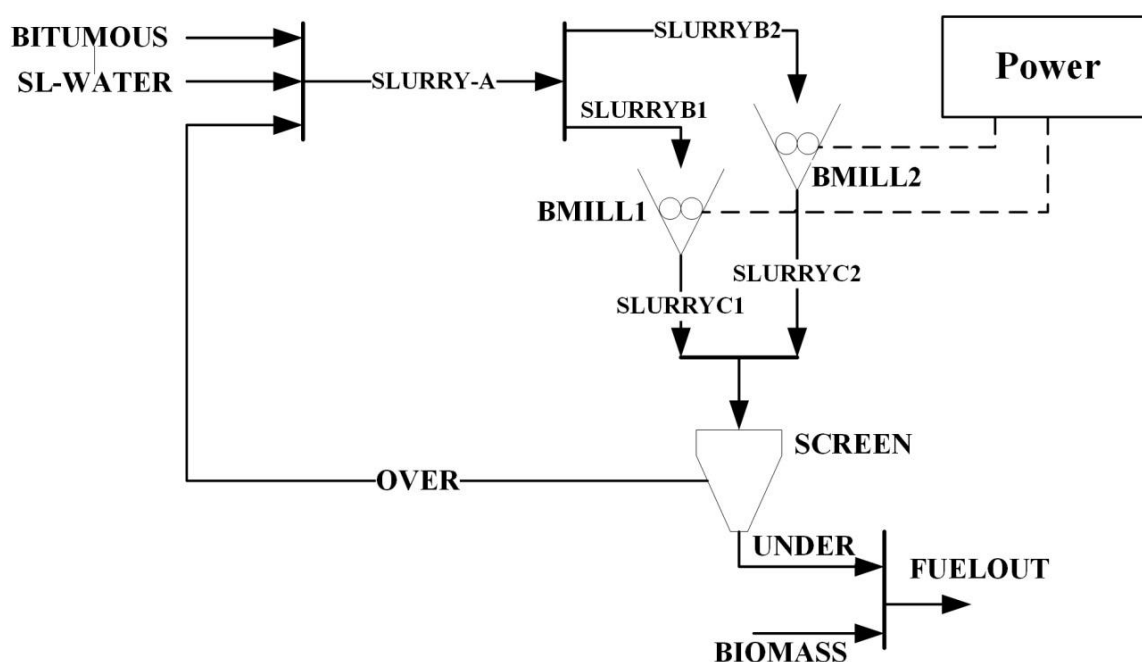


Figure 2. simulation of coal sizing unit block diagram by Aspen software

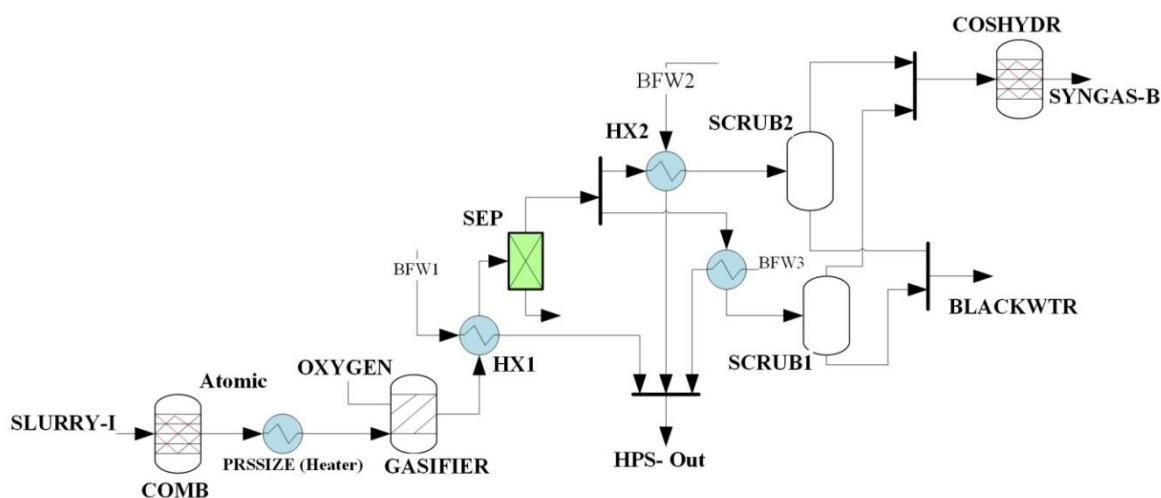


Figure 3. Simulation of overall schematic of coal gasification unit by Aspen software

Table 6. Comparison of Gibbs and kinetic equilibrium models with experimental data in the gasifier reactor

Case #		1	2	3	4	5	6	7	8
Average pressure	bar	1.6	1.55	1.55	1.65	1.45	1.45	1.55	1.01
Average temperature	oC	810	880	850	780	870	840	810	750
Coal feed rate	kg/h	26.4	19.2	25.0	30.9	19.4	24.8	29.8	24.7
Air supply rate	kg/h	68	70	71	69	74	74	70	54
Air ratio	±	0.37	0.52	0.41	0.32	0.54	0.42	0.33	0.31
Superficial velocity	m/s	6.0	6.8	6.7	5.9	7.6	7.4	6.5	7.2
Measured dry gas composition:									
CO	%	10.2	9.1	12.0	13.4	10.1	13.2	13.6	9.7
CO ₂	%	15.7	15.0	13.1	13.3	14.2	12.3	13.0	15.5
H ₂	%	8.0	5.6	8.5	10.4	5.6	8.4	9.9	8.8
CH ₄	%	1.0	0.5	0.8	1.0	0.5	0.8	1.0	1.0
N ₂	%	65.1	69.8	65.6	61.9	69.6	65.3	62.5	65.1
Dry gas yield	kg/kg	3.1	4.1	3.3	2.7	4.3	3.4	2.8	2.6
Dry gas HHV	MJ/Nm ³	2.6	2.0	2.8	3.3	2.1	2.9	3.3	2.7
Carbon conversion	%	61.4	73.8	65.2	56.2	77.4	68.1	58.8	51.1
Predicted dry gas composition:									
(a) Assuming that carbon conversion is determined only by equilibrium									
CO	%	8.2	8.2	10.4	12.6	10.6	13.2	12.9	10.0
CO ₂	%	16.3	16.2	15.1	13.9	14.9	13.5	13.7	15.4
H ₂	%	10.4	8.0	10.3	13.0	8.3	10.8	12.8	13.1
CH ₄	%	0.9	0.5	0.6	0.8	0.4	0.5	0.8	0.9
N ₂	%	64.1	67.0	63.5	59.6	65.7	62.0	59.7	60.5
Dry gas HHV	MJ/Nm ³	2.5	2.1	2.6	3.3	2.3	2.9	3.2	3.0
T _{0eq}	K	860	860	880	900	860	900	900	840
T _{0eq} - T _{0ave}	K	-220	-290	-240	-150	-280	-210	-180	-180
$\Sigma(Y_{eq} - Y_{meas})^2$	%	11.4	15.7	13.9	13.0	17.5	17.7	17.4	26.2
(b) After introduction of a kinetic carbon conversion									
CO	%	13.9	11.5	12.9	13.4	10.7	13.3	13.6	12.5
CO ₂	%	13.0	12.3	13.7	12.7	14.2	12.6	12.5	13.3
H ₂	%	9.9	6.7	9.4	11.9	6.4	8.6	11.4	12.7
CH ₄	%	0.0007	0.0001	0.01	0.002	0.0003	0.0004	0.002	0.02
N ₂	%	63.9	68.1	64.7	62.1	68.8	65.4	62.3	61.4
Dry gas HHV	MJ/Nm ³	2.8	2.1	2.0	2.9	2.0	2.6	2.9	3.0
T _{0eq}	K	1000	1080	1060	1080	1100	1120	1100	1020
T _{0eq} - T _{0ave}	K	-80	-70	-60	30	-40	10	20	0
$\Sigma(Y_{eq} - Y_{meas})^2$	%	24.4	9.7	2.9	3.4	2.7	0.8	3.2	39.5

In this section, reactions are divided into three groups of reactions decomposition of coke, biomass feedstock, gasification and hydrolysis of carbonyl sulfide. Gasification process begins with decomposition (pyrolysis) and continues with combustion. Therefore, the feed into this section is initially introduced into the Comb reactor, and there decomposition of feedstock reactions are carried out. RStoic model is used for this purpose. The stoichiometric coefficients of these reactions are the function of feedstock characteristics and determine the yields of the products. In coal gasification, if the design determination is just to design the reactor alone and to carefully examine the behavior of its components, kinetic models are used, but when it is used in conjunction with other units and in the form of flow sheet, the Gibbs model is used. In similar cases, the same model has been used and shown that the results with the experimental reactor have small differences and acceptable (X. Li et al., 2001).

This comparison, which is performed using the "sum of squared data difference", firstly, kinetic and equilibrium results are similar to each other, and secondly, they are close to the experimental data in Table 5. Therefore, in this study, a suitable model for the gasifier unit is based on the minimum Gibbs free energy and equilibrium state and it is assumed that the residence time is long enough to give the reactions the opportunity to reach the equilibrium; the corresponding model is in the RGibbs software environment. Therefore, the feedstock enters into the gasifier reactor for gasification reactions. The output of this reactor has a high temperature and it is cooled by boiling saturation water. The reactor outlet after passing through the heat exchangers and heat transferring is entered in to the scrubbers so that by direct contact to water separate out as a solvent of dust particles and toxic gases from the produced gases. The exhaust gases from the gasifier reactor enter the cyclone and associated solid particles are separated from

the gas stream. In the end, the main stream of the process enters to the COSHYDR reactor, and the hydrolysis of carbonyl sulfide is carried out. The RStoic model has been employed for performing of reaction.

There are assumptions for simulating of this section such as:

- Models are steady-state and non-kinetic and isothermal.
- Chemical reactions occur in a state of equilibrium in gasifier, and the pressure drop is negligible.

- All components, with the exception of sulfurs, are involved in the chemical reaction.
- All gases are ideal (including hydrogen, carbon monoxide, carbon dioxide, water vapor, nitrogen and methane)
- Coal contains only carbon and ash in solid phase.

2.3.3. Simulation of Gas cleaning Unit

The gas produced from the gasification unit is initially cooled, which supplies part of its energy through the exchange of heat with refined syngas.

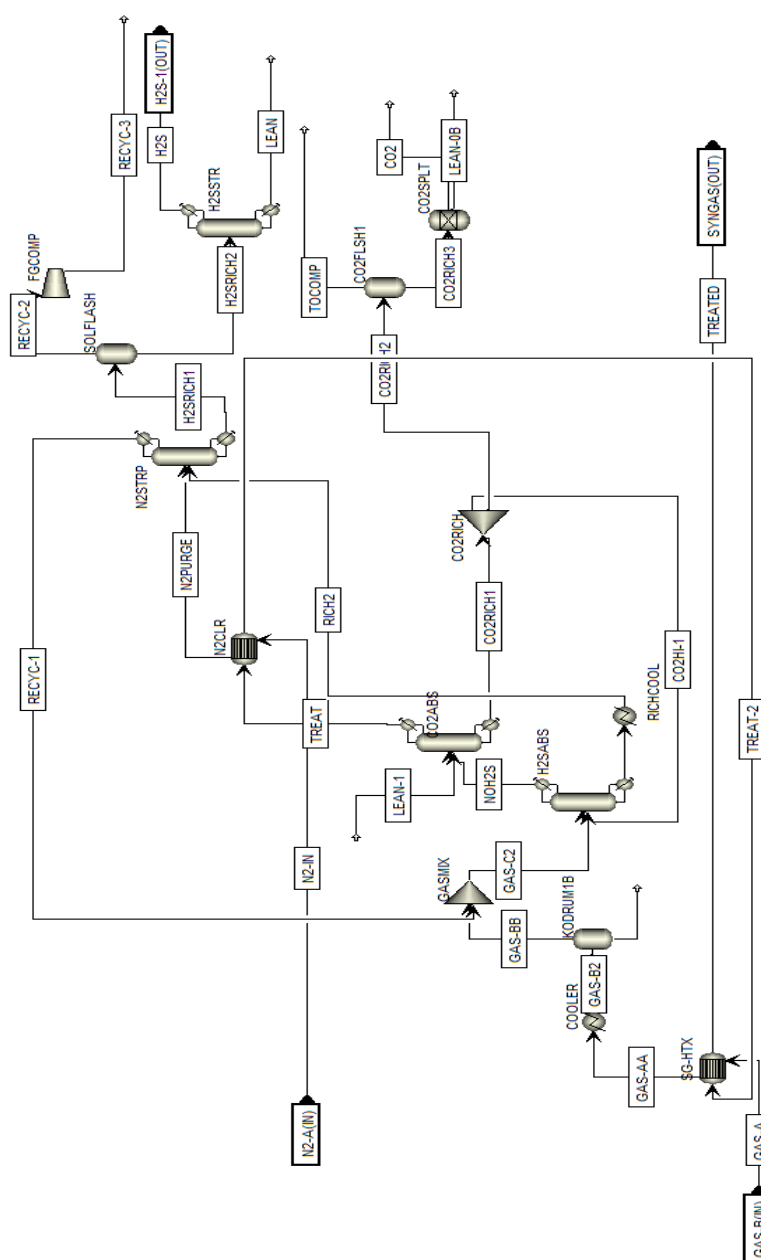


Figure 4. Simulation of developed flow diagram of syngas treatment by Aspen software

The water along with some acid and nitride compounds is removed from the separator in liquid form, and the resulting gas is mixed with returned gas from nitrogen stripper. Next it enters to the absorption system of H₂S and contacts with the solvent of the absorber tower and absorbs the H₂S, and then the free H₂S stream enters the second absorption tower and is absorbed by its CO₂ solvent. The H₂S rich solvent stream is sent to the nitrogen stripper, and with the aid of nitrogen flow, the light components are along with the residual CO₂ are separated. The H₂S rich stream is sent to the stripper tower and H₂S is removed from the solvent and the solvent is returned to the absorption cycle and its H₂S can be sent to the Claus unit. Fig. 4 illustrates the schematic of overall process in this section.

2.3.4. Simulation of Power Generation Unit

Power generation unit is one of the major units affecting on process economic, so its appropriate integration with the whole process has a great impact on operating costs. Nowadays, due to the extensive capabilities of commercial software, especially Aspen Plus software, there are good and accurate models of equipment such as steam turbines and gas turbines in the software that allow to simulate

accurately the power generation units (Dlugosel'skii et al., 2007; Hlavacek et al., 1994; Ligang Zheng & Furimsky, 2003).

The produced and refined gas from the Gas Cleaning Unit is divided into three parts, and one part is fed into the power and electricity generation unit, and other parts of the produced gas are fed into WGS and FT units. That how the distribution of produced gas between units and how much gasification should be included in the production unit can then be determined with the economic optimization of the system. The syngas firstly enters into the combustion chamber in the power generation unit, where combustion has been occurred using compressed air, and then the exhaust gases from the combustion chamber enter the gas turbine and provide mechanical power. Since the Tail Gas output from the Fischer-Tropsch unit is containing light hydrocarbons predominantly C₁ to C₅, it is better to enter into the power generation unit and generate electricity through a gas turbine. But since the Tail Gas pressure from the Fischer Tropsch unit is different with syngas pressure output from the gas cleaning unit, so a gas turbines for the Tail Gas in the power generation unit is considered.

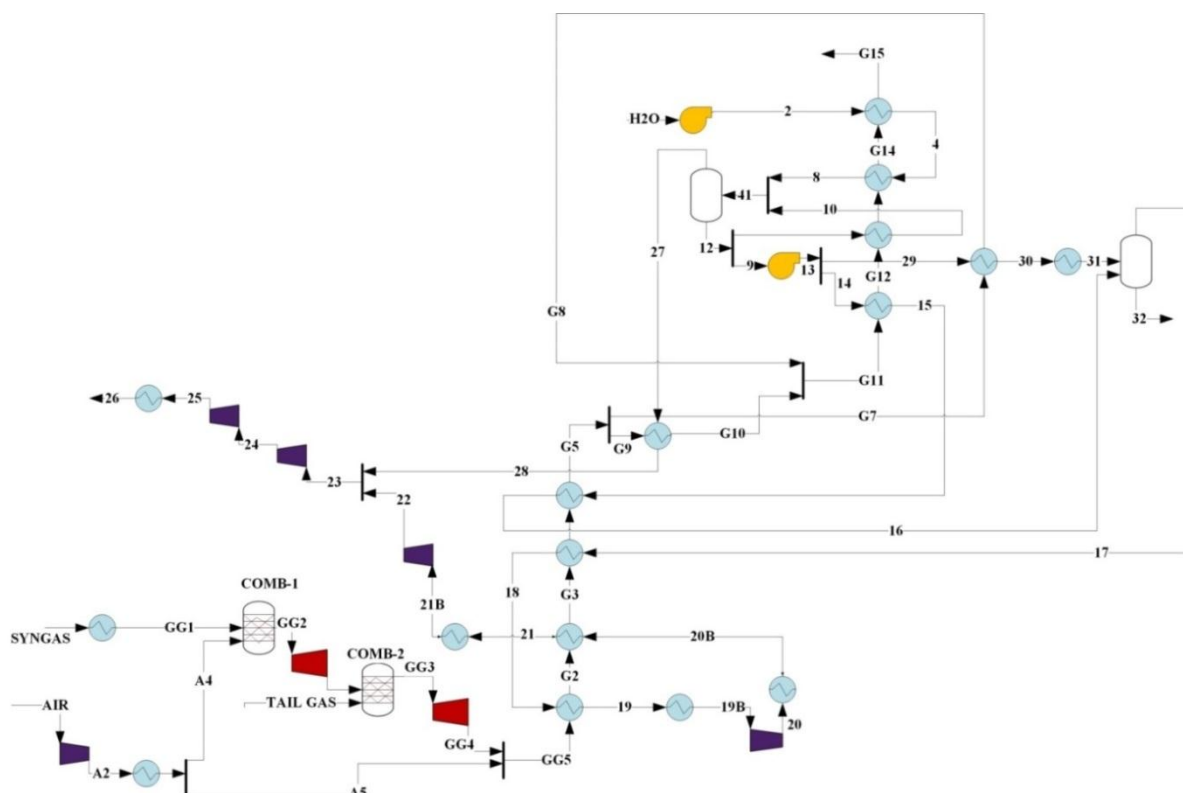


Figure 5. Simulation of power generation unit by Aspen software

The exhaust gases from gas turbine are mixed with tail gas from the FT unit and enter to combustion chamber of the gas turbine of the associated gases, and mechanical power also is produced in this section. The output of the second gas turbine has a temperature of about 700 °C, which can use from heat and produce steam at different levels. This steam is used for steam turbine circulation and produces more mechanical work. Fig. 5 is an illustration of this unit. In this process, the hot gases of the gas turbines have been employed to produce steam at four pressure levels, including high steam pressure 162.9 bar, high pressure steam 39 bar, medium pressure 27.6 bar steam and low pressure steam 3 bar. In order to maximize the production capacity of this unit, a condensing steam turbine is used, where the low pressure steam at pressure of 3 bar is entered into the last turbine, and its output under vacuum is entered into the condenser.

2.3.5. Simulation of WGS

A part of the gas produced from the gasification unit after treatment is entered into the unit to convert CO to CO₂. In this

way, ratio of hydrogen to carbon monoxide (H₂ / CO) is increased to provide the gas ratio required for the Fischer-Tropsch process. Because the shift reaction is endogenous, in order to maximize the conversion rate, the output from the first reactor is cooled and enters into the second reactor.

The lower streams of CO₂ absorption tower is used to cool the outlet stream of the reactors. In this process, due to the fact that part of CO is converted into CO₂, absorption system with solution is used to purify the exhaust gas from the reactors. The output of the second reactor after the initial cooling with the lower stream of the absorption tower is exchanged heating again with the upper stream of the tower to cool down and then enter to the CO₂ absorber tower. In this tower, the existing CO₂ is absorbed by solvent and the hydrogen stream is produced without CO₂. This stream can be mixed with a portion of the purified syngas from gasification unit and enters into the Fischer-Tropsch process with H₂ to CO ratio of 2. A schematic of the process is presented in Fig. 6.

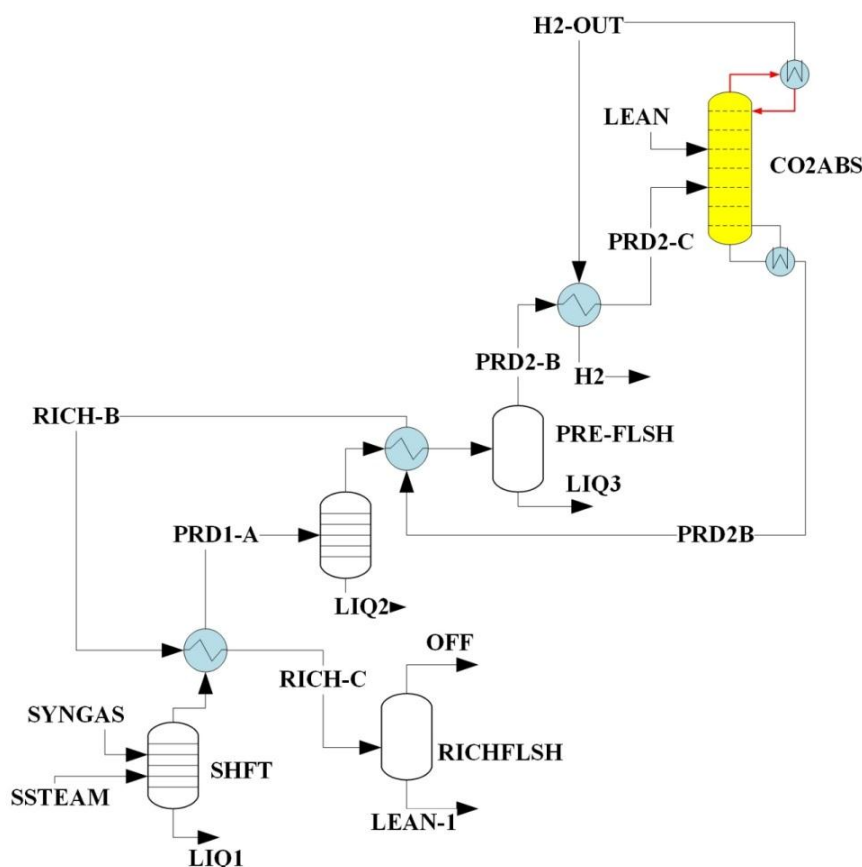


Figure 6. Simulation of water-gas shift (WGS) unit by Aspen software

2.3.6. Simulation of the Oxygen Production Unit by Air Separation

Three different commercial methods are used for air separation: cryogenic distillation, pressure swing adsorption (PSA), and membrane process. In the process of cryogenic distillation, the purity of commercial produced oxygen is 99.5% and its nitrogen is regarded as a byproduct, but if it is desired, nitrogen can be obtained with a purity of 99.99%.

In the pressure swing adsorption process, activated carbon is used for nitrogen recycling, and absorbent materials are based on synthesized zeolites used in oxygen adsorption. This process can be competitive with the cryogenic distillation process if required purity and volume are exceeded to 95% and 100 tons per day, respectively. The membrane technology of hollow fibers has been developed rapidly for air separation. These systems are commercially available for the recovery of nitrogen. Due to the fact that pressure swing adsorption and membrane methods are more cost effective in low capacities of oxygen production, hence, in the present project, considering the high capacity of the feed, the cryogenic distillation method has been selected. Fig. 7 shows the schematic of the simulation of air separation unit as well as supplying of oxygen and nitrogen gases required for the gasification and gas treatment process.

In this process, after four stages of compression, the air pressure is increased from 1 to 6.3 bar. The moisture content is taken up to a certain extent before compressing, and the moisture content is completely taken after final compression. Then the flow of air is divided into two parts with a ratio of 95% and 5%, and these flows are compressed in heat exchanger and.

The streams are mixed and exchanged heat with oxygen and nitrogen streams generated from the distillation tower. The main branch of the air flow in this exchange reaches to temperature of -170°C and the other branch reaches to the temperature of -132°C , then the air at the temperature of -170°C enters to the distillation tower and the second branch of air reaches to temperature of -132°C and enters into the turbo-expander and its pressure is reduced to 1.9. In this pressure reduction, the air temperature reaches to -163°C , and then this branch of air is entered into the tower. Oxygen with 95% purity and nitrogen with 99.6% purity are exited streams from cryogenic distillation tower. These streams exchange heat with inlet air flow, and then the oxygen flow reaches 41 bar with several stages of compression, which is ready to be fed to the gasification unit. Nitrogen flow reaches 27 bar after several compression stages and is fed to the Gas Cleaning unit.

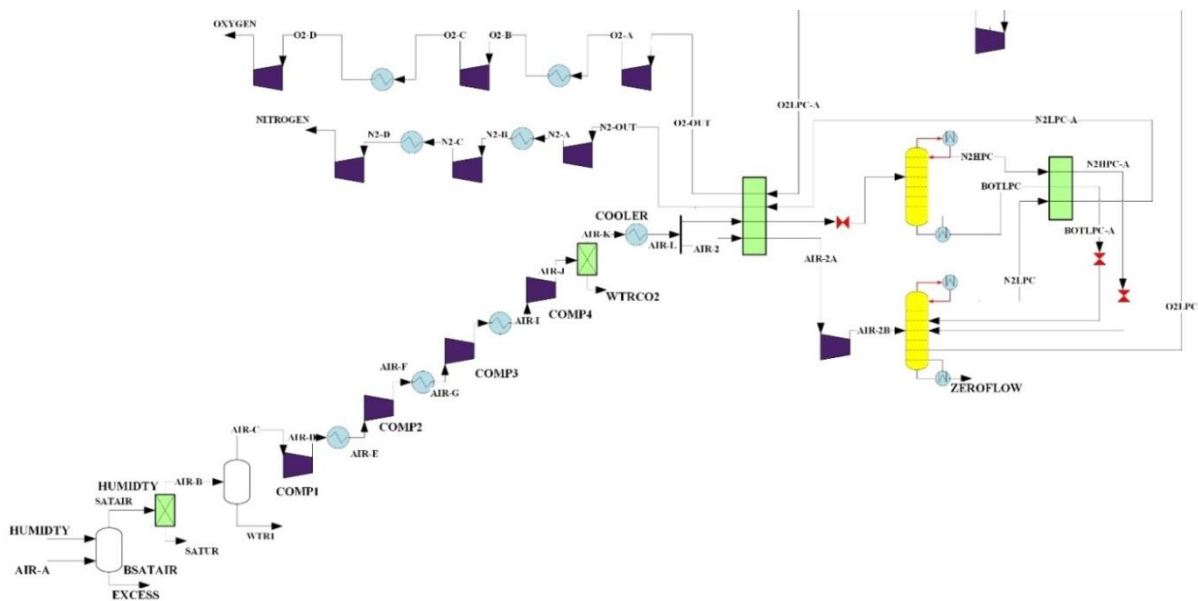


Figure 7. Simulation of Air separation unit (ASU) by Aspen software

2.3.7. Simulation of Fischer-Tropsch Unit

In a CTL process, the Fischer-Tropsch synthesis unit is the main unit, and its reactor is the heart of the whole process. The refined syngas from gasifier unit has the ratio of H_2/CO approximately equal to 0.67 which is mixed with the stream of hydrogen from the WGS unit and provides the H_2/CO ratio of 2, which is suitable for the Fischer-Tropsch process. This process is carried out at the temperature of about 240 °C and the pressure of about 20 bar, and the syngas is mainly converted to hydrocarbons from C1 to C30 and water. In fact, the growth of the hydrocarbon chain in the Fischer-Tropsch process depends on the operating conditions and the catalyst, and it can lead to heavier hydrocarbons than the C30. Since the database of software does not contain hydrocarbons that are heavier than the C30, chemical reactions are thus defined up to C30. The input syngas stream,

entered into the unit, with the stream of the exhaust from the reactor exchanges heat, and then it enters to the Fischer-Tropsch reactor. Because of the high heat generated by the process for the isothermal process, saturation water is used to control the temperature of the reactor. The generated heat in the reactor leads to vaporizing of saturation water; consequently it is converted into water vapor, which can later be used to generate power.

The products of the Fischer-Tropsch reactor are converted to lightweight liquids, heavyweight (wax) liquids and associated gases with the help of gradual cooling in the three separators. Lightweight and heavyweight hydrocarbons liquids are considered as the main products of the process, and associated gases are sent to the power plant to enter the gas turbine for power generation. Fig. 8 shows the flow diagram of the Fischer-Tropsch unit.

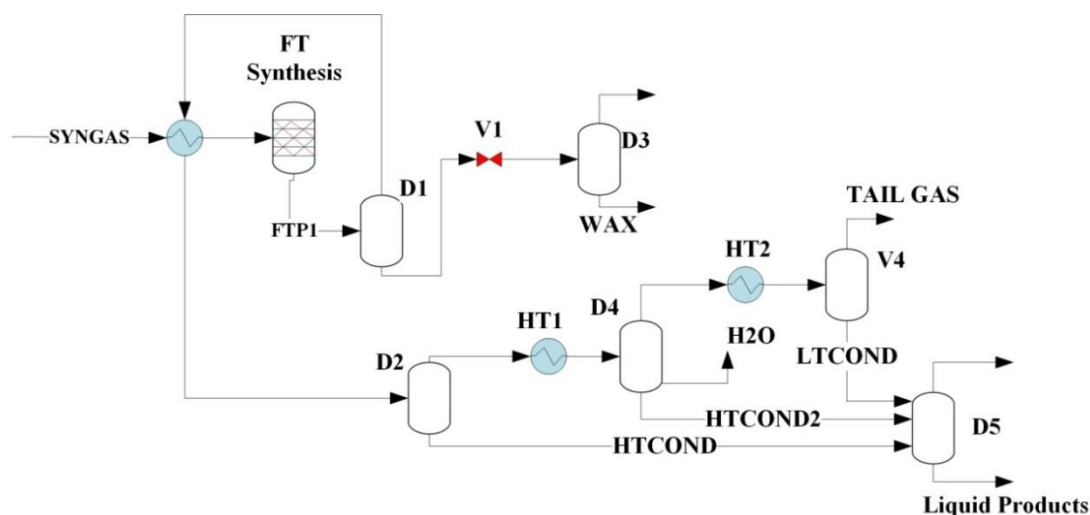


Figure 8. Simulation of Fischer-Tropsch unit by Aspen software

Table 7. Properties of some heat exchangers of process

Name	Efficiency (polytropic/isentropic) used	Calculated discharge pressure (bar)	Calculated pressure change (bar)	Calculated pressure ratio	Outlet temperature (°C)	Isentropic outlet temperature (°C)	Isentropic power requirement (kW)
ASU.COMP1	0.72	1.99948	0.98623	1.97333	93.8938	70.5254	8164.16
ASU.COMP2	0.72	3.69973	1.70025	1.85034	114.514	91.9221	7921.53
ASU.COMP3	0.72	5.19865	1.49892	1.40514	76.5347	64.5452	4203.97
ASU.COMP4	0.72	6.3	1.10135	1.21185	60.1858	53.5099	2344.04
ASU.GOXCMP-1	0.72	6.52906	5.42906	5.93551	267.921	198.694	5537.75
ASU.GOXCMP-2	0.72	23.0765	16.5474	3.53443	215.749	166.957	3900.09
ASU.GOXCMP-3	0.72	41.0028	17.9264	1.77682	110.355	90.5588	1587.83
ASU.N2CMP-1	0.72	5.51581	4.41581	5.01437	243.891	179.925	17424
ASU.N2CMP-2	0.72	20.6843	15.1685	3.75	230.074	176.387	14738.6
ASU.N2CMP-3	0.72	27.579	6.89476	1.33333	71.5432	61.692	2738.11
ASU.TURB-1	0.72	1.90114	-4.29886	0.306635	-163.367	-173.69	-254.775
ASU.TURB-2	0.72	1.2	-2.18899	0.354087	-181.768	-181.772	-765.392
CLEANING.FGCOMP	0.72	27.579	20.6843	4	123.385	80.2835	24.4191

Name	Efficiency (polytropic/ isentropic) used	Calculated discharge pressure (bar)	Calculated pressure change (bar)	Calculated pressure ratio	Outlet temperature (°C)	Isentropic outlet temperature (°C)	Isentropic power requirement (kW)
FT.ST-02	0.86	7	-21.0608	0.249458	165.709	165.709	-10055.6
GASFR.ST-01	0.86	60	-71.6899	0.455616	274.915	274.915	-12048.3
POWER.COMP	0.912	30	28.987	29.615	536.838	466.095	82361.7
POWER.EXP1	0.877	16.8	-12.0003	0.583327	1298.66	1273.82	-50856.6
POWER.EXP2	0.86	1.04939	-15.0806	0.065058	698.478	588.568	-208127
POWER.HPTURB	0.865	40.5478	-121.387	0.250396	357.322	335.142	-13201
POWER.IP1	0.9	7.28748	-31.7398	0.186728	325.57	300.304	-16808.9
POWER.IP2	0.89	3.08168	-3.19255	0.491164	242.837	233.226	-6576.01
POWER.LP	0.875	0.067569	-3.01411	0.021926	38.368	38.368	-23389.6

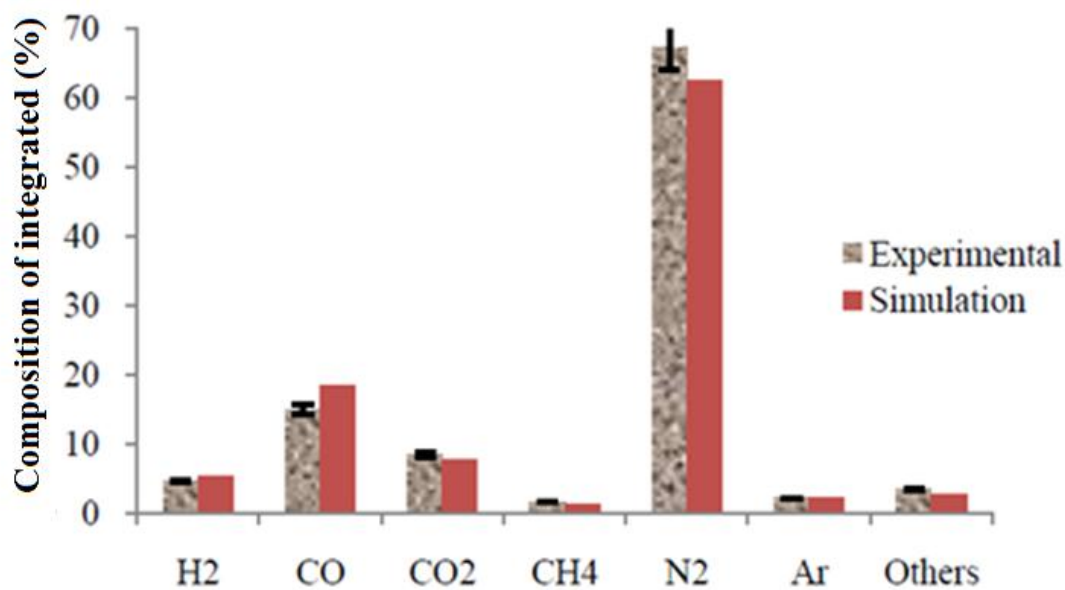


Figure 9. Comparison of results of gasifier model in this paper with empirical data in referenced paper

2.3.8. Comparison of Simulation Results of Gasifier with an Empirical Work

The proper model for the gasifier is based on the minimization of Gibbs free energy and in equilibrium state, and it is assumed that the residence time is long enough to give the reactions the opportunity to achieve equilibrium state. This model has been developed in the software environment, and therefore it is appropriate to compare with an empirical work.

In Fig. 9, the results of this research model were compared with the empirical data presented in (Dlugosel'skii et al., 2007; Hlavacek et al., 1994; Ligang Zheng & Furimsky, 2003); they used this model for gasification of solid municipal waste. The results show that the results are in good agreement with the experimental data, and the error of composition percentage of syngas

emitted from the gasifier with the experimental data is about 4%.

3. Sensitivity Analysis

Sensitivity analysis is used as a powerful tool to understand the effect of several key variables of the model. Since the developed process model in this study has a lot of complexity, mass and energy connections between process units are very high, so before the study of the sensitivity analysis, determining of objective function or cost function is the first step. In the present study, the extended objective function, "Gross profit from the sale of electrical power and hydrocarbon products" is considered, and feed costs are not included in the calculations, so the objective function of the study will be as follows:

$$\text{Obj. Fun} = \sum_i C_i \times \text{Power Generation}_i + \sum_j C_j \times \text{Products}_j \quad (1)$$

In Equation 1, the coefficients C_i and C_j are respectively the unit price of sales of power (commercial electricity) and hydrocarbon product.

In the present article, with the help of Aspen Plus software sensitivity analysis tool, the effect of the most important operational variables on the objective function is studied. The following figure shows the block diagram of the developed process model. One of the most important variables affecting the process is the distribution of syngas

production among the power generation, fuel and WGS units. In general, since the output of this distributor is divided into three parts, the system's degree of freedom is equal to 2, but because the input ratio of H_2/CO to the Fischer-Tropsch unit should be equal to 2. Therefore, this process limitation decreases the degree of system freedom, and the degree of freedom of the syngas distribution system will be equal to one, and the rest of the ratios will be calculated by determining the amount of syngas which should enter into the production unit. Solving the above problem at the same time with the problem of sensitivity analysis is a sample of the aforementioned complexities.

Table 8. Properties of some compressors and turbines of process

Name	Efficiency (polytropic/isentropic) used	Calculated discharge pressure (bar)	Calculated pressure change (bar)	Calculated pressure ratio	Outlet temperature (°C)	Isentropic outlet temperature (°C)	Isentropic power requirement (kW)
ASU.COMP1	0.72	1.99948	0.98623	1.97333	93.8938	70.5254	8164.16
ASU.COMP2	0.72	3.69973	1.70025	1.85034	114.514	91.9221	7921.53
ASU.COMP3	0.72	5.19865	1.49892	1.40514	76.5347	64.5452	4203.97
ASU.COMP4	0.72	6.3	1.10135	1.21185	60.1858	53.5099	2344.04
ASU.GOXCMP-1	0.72	6.52906	5.42906	5.93551	267.921	198.694	5537.75
ASU.GOXCMP-2	0.72	23.0765	16.5474	3.53443	215.749	166.957	3900.09
ASU.GOXCMP-3	0.72	41.0028	17.9264	1.77682	110.355	90.5588	1587.83
ASU.N2CMP-1	0.72	5.51581	4.41581	5.01437	243.891	179.925	17424
ASU.N2CMP-2	0.72	20.6843	15.1685	3.75	230.074	176.387	14738.6
ASU.N2CMP-3	0.72	27.579	6.89476	1.33333	71.5432	61.692	2738.11
ASU.TURB-1	0.72	1.90114	-4.29886	0.306635	-163.367	-173.69	-254.775
ASU.TURB-2	0.72	1.2	-2.18899	0.354087	-181.768	-181.772	-765.392
CLEANING.FGCOMP	0.72	27.579	20.6843	4	123.385	80.2835	24.4191
FT.ST-02	0.86	7	-21.0608	0.249458	165.709	165.709	-10055.6
GASFR.ST-01	0.86	60	-71.6899	0.455616	274.915	274.915	-12048.3
POWER.COMP	0.912	30	28.987	29.615	536.838	466.095	82361.7
POWER.EXP1	0.877	16.8	-12.0003	0.583327	1298.66	1273.82	-50856.6
POWER.EXP2	0.86	1.04939	-15.0806	0.065058	698.478	588.568	-208127
POWER.HPTURB	0.865	40.5478	-121.387	0.250396	357.322	335.142	-13201
POWER.IP1	0.9	7.28748	-31.7398	0.186728	325.57	300.304	-16808.9
POWER.IP2	0.89	3.08168	-3.19255	0.491164	242.837	233.226	-6576.01
POWER.LP	0.875	0.067569	-3.01411	0.021926	38.368	38.368	-23389.6

Table 9. Properties of some reactors of process

Name	Property method	Specified pressure (psia)	Specified temperature (°C)	Specified heat duty [Btu/hr]	Outlet temperature (°C)	Outlet pressure (bar)	Calculated heat duty (Gcal/hr)	Net heat duty (Gcal/hr)
NCCHNG	PENG-ROB	14.6959	-	0	55.8066	1.01325	0	0
FT.FT	PENG-ROB	275.572	240	-	240	19	-61.2607	-61.2607
GASFR.COMB	PENG-ROB	0	15.5556	-	15.5556	1.01325	274.553	274.553
GASFR.COSHYDR	PENG-ROB	0	-	0	152.442	27.579	0	0
POWER.COM2	STEAM-TA	-9.7175	-	0	1350.03	16.13	0	0
POWER.COMB-A	PR-BM	-17.4	-	0	1474.27	28.8003	0	0

The impact of the syngas distributor on the objective function can be assessed using the sensitivity analysis tool. Considering the great integration in the developed process model, the entire site can be evaluated with the help of this variable. For example, with the increase of syngas entrance into the fuel production unit, the share of liquid hydrocarbon production is increased, but the share of gas synthesis consumed by the unit of power production is reduced. Since the share of gasification of the Fischer-Tropsch unit is increased as much as the share of the associated gases produced in Fischer-Tropsch unit; consequently, these associated gases are re-fed to power generation units and generate electricity.

Fig.10 shows the effect of gas distribution on hydrocarbon production and power generation. As shown in the figure, with the increase in the amount of gas entrained into the power generation unit, the share of the production of fuel is reduced and the share of power generation is increased. The important

thing is that, by pushing the gas distribution into the power sector to zero, the power output does not go to zero. Because part of the production capacity of this unit is obtained from associated gases of Fischer-Tropsch and steam turbines from the steam generator of Fischer-Tropsch and gasification reactor. But by pushing the gas distribution into the power sector to 100%, the share of fuel production is going to be zero, which is consistent with the reality of the problem.

The most important parameter in the objective function i.e. equation 1, which has uncertainty, is the coefficients C_i and C_j , which represent the price of electricity sales and hydrocarbon products, respectively. Figure 11 shows the effect of the distribution of gas into the power generation sector on the objective function. In the presented sensitivity analysis, it is assumed that the electricity cost per kilowatt-hour is 4.2 Cent and the price of hydrocarbon products is \$ 50 per barrel.

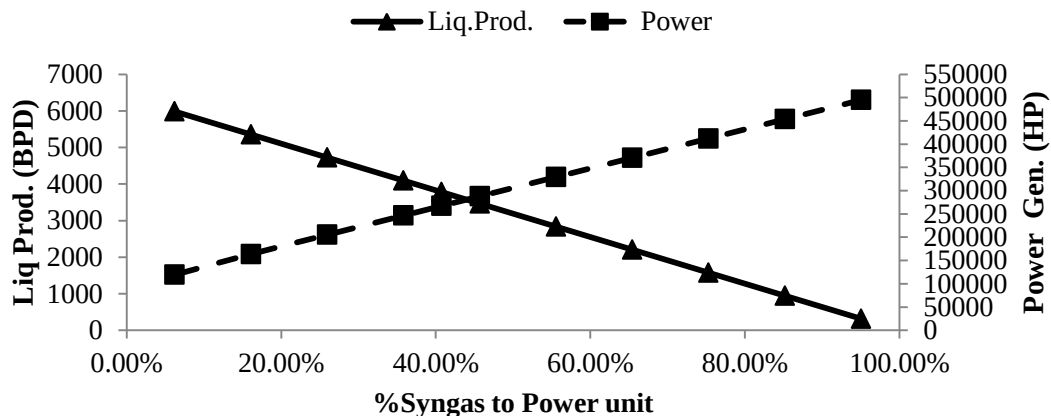


Figure 10. The effect of the synthesis gas distribution in the production of products

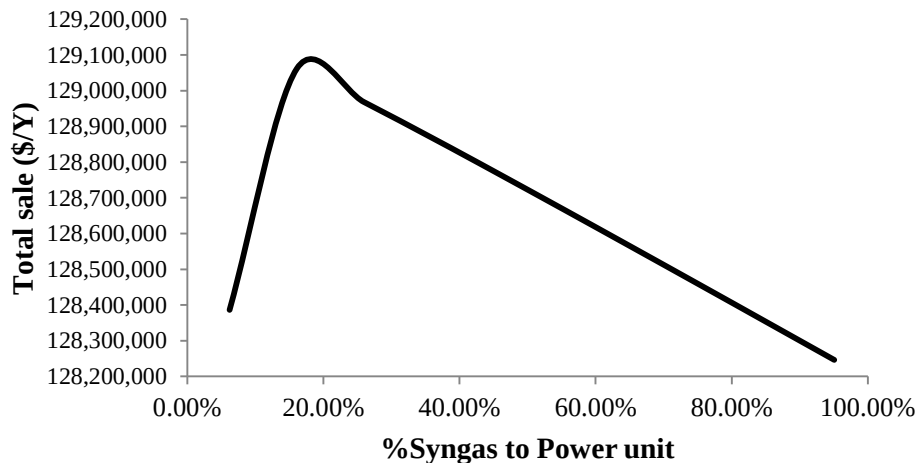


Figure 11. The effect of gas distribution on the objective function (the price of electricity is 4.2 Cent per kilowatt-hour and the price of liquid fuel sales of Fischer-Tropsch is 50 USD per barrel)

According to the abovementioned assumptions, Fig. 11 shows that the gas optimal distribution point entered into the power generation sector is approximately equal to 16%. The calculations show that if 16% out of the total production of syngas is entered into the power generation sector and 42.5% of it enters into the Fischer-Tropsch unit and the rest of it i.e. 41.5% is employed to set the H₂/CO ratio entered into the WGS unit, the annual gross profit will be the highest amount in this case. The point to be considered is in the form of changes in the objective function. As it can be seen with assumed prices, the range of changes in the objective function is about 1 million USD per year.

If we analyze the sensitivity of the hypothesized prices, then the following figure is obtained where the selling price of liquid hydrocarbon products is assumed to be 50 USD per barrel and the price of electricity sales varies from 2.1 Cent to 8.4 Cent per kWh.

Because of the wide variation in the objective function in the other tariff, the range of changes for tariff of 4.2 Cent per kilowatt-hour is not tangible. Fig. 12 shows that if the sales price of electricity reaches more than 4.2 Cent per kilowatt hour, the fuel production unit should be removed from the production and all of the production of syngas is sent to the production unit, and if the price of

electricity sales is less than 4.2 Cent per kWh, it is better to send all the produced syngas to the fuel production unit, and the power generation unit only is fed by the associated gasses and steam produced by Fischer-Tropsch and Gasification. It should be noted that the result of this section is assumed based on 50 USD per barrel of liquid fuel.

Now, if the selling price of electricity equals to 4.2 Cent per kilowatt-hour and assumed constantly while the price of liquid hydrocarbon products is variable, because of the wide variation in the objective function in the other tariffs, the range of changes for the tariff of 50 USD per barrel of liquid fuel is not tangible.

Fig. 13 shows that if the sales price of hydrocarbon products reaches less than 50 USD per barrel, the fuel production unit should be removed from production and all of the production of syngas is sent to the production unit, and if the sale price of hydrocarbon products exceeds 50 USD per barrel, it is better to send all the produced syngas to the fuel production unit, and the power generation unit only is fed by the associated gasses and steam produced by Fischer-Tropsch and Gasification. It should be noted that the result of this section is assumed at a price of 4.2 Cent per kilowatt-hour.

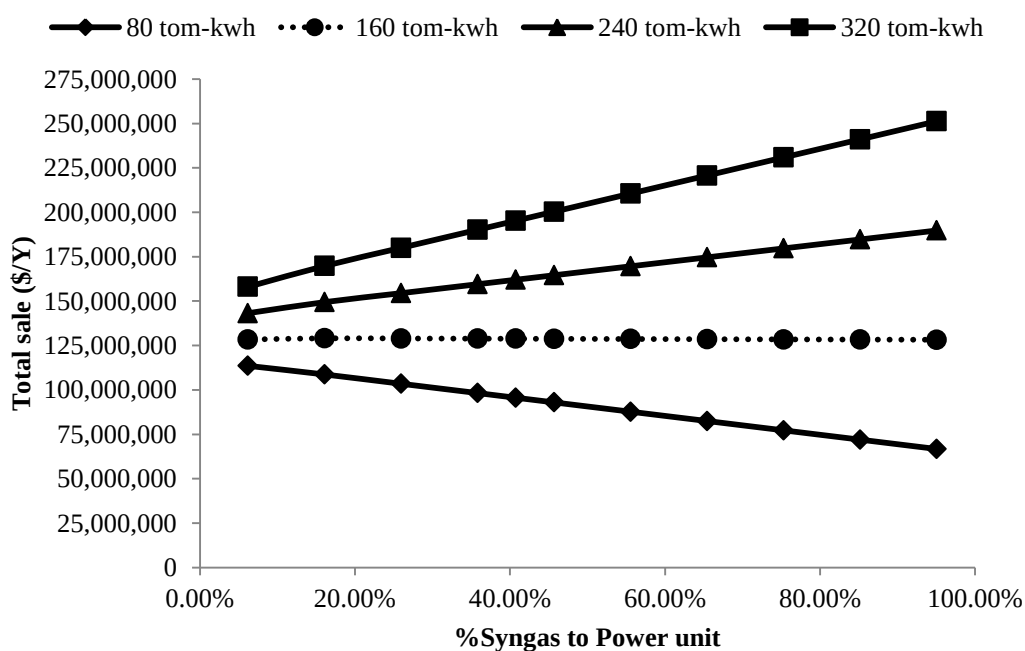


Figure 12. Impact of syngas distribution and uncertainty of the sale price of products on the objective function (electricity price of 50 USD per kilowatt hour)

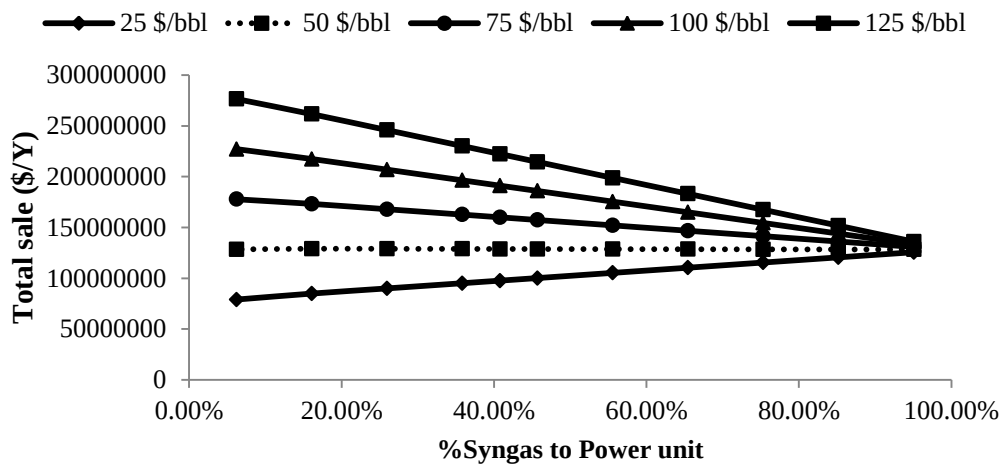


Figure 13. Impact of syngas distribution and uncertainty of the sale price of products on the objective function (electricity price of 4.2 Cent per kiloWatt hour)

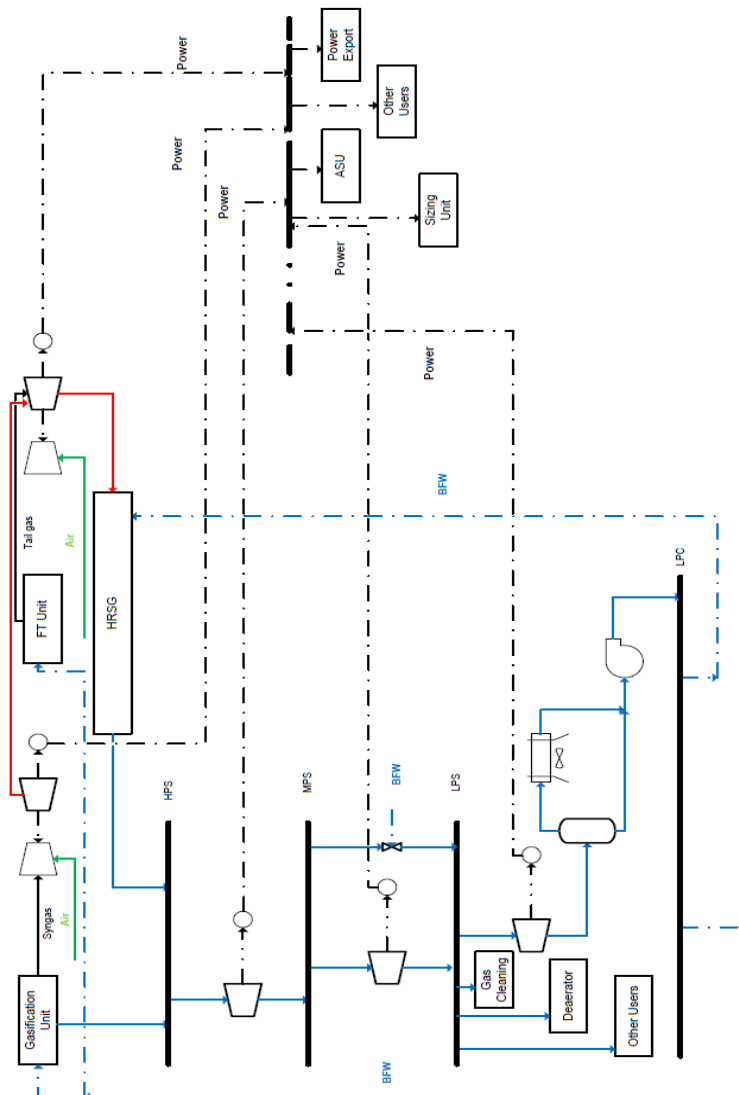


Figure 14. Integration of power and heat in CHPF process

Fig. 14 shows the thermal and power relationships of process units. As it can be seen in the figure, the integration of each unit is independently observed and the excess heat potential of the units is employed for steam generation. The steam is used for preheating of the coolant water of the Fischer-Tropsch reactor, boiling of reboilers in process units, and the propulsion power of compressors and choppers. In addition, part of the steam generating by power generation unit along with the production capacity of the gas turbines can be used for sale.

Conclusion

In this paper, considering of an integrated gasification combined cycle (IGCC) plant with input feed of coal, an integrated system of "Combined heat and power as well as liquid fuel of Fischer-Tropsch", called CHPF, is designed and simulated. Using an objective function the optimum amounts of production of the power, heat and liquid fuel are provided at a certain scale of the feedstock. Due to the novel design of the gas system, the results were compared with an experimental work and showed that the difference in results was about 4%, which is acceptable amount. In general, the findings of this research can be summarized as follows:

- Integrated design of the CHPF process as an entirely new superstructure with the development of upstream and downstream units and the impact of individual operating units on the overall system performance.
- Simultaneous production of heat, power and liquid fuel of Fischer-Tropsch with the combination of IGCC and FT units and their simultaneous impact on process economics by examining the effect of the price of energy and fuel carriers on the process efficiency and determining the optimal point of work by changing tariffs.
- Performing the combined heat and power integration for the whole process, taking into account process and operational constraints, and examining the changing operating conditions on the efficiency of total system efficiency and energy
- Using the conceptual method of sensitivity analysis of the results and analyzing the uncertainty of the model in order to confirm the design results and better cognition of designed cycle show that the best point for distributing syngas to the power generation unit is about 16% based on the expected objective function.

References

- Aghaie, M., Mehrpooya, M., & Pourfayaz, F. (2016). Introducing an integrated chemical looping hydrogen production, inherent carbon capture and solid oxide fuel cell biomass fueled power plant process configuration. *Energy Conversion and Management*, 124, 141-154.
- Algieri, A., & Morrone, P. (2014). Energetic analysis of biomass-fired ORC systems for micro-scale combined heat and power (CHP) generation. A possible application to the Italian residential sector. *Applied Thermal Engineering*, 71(2), 751-759.
- Amidpour, M., Panjeshahi, M. H., & SHARIATI, N. M. (2009). Energy optimization in gas-to-liquid process.
- Asadullah, M. (2014). Biomass gasification gas cleaning for downstream applications: A comparative critical review. *Renewable and sustainable energy reviews*, 40, 118-132.
- Athari, H., Soltani, S., Bölükbaşı, A., Rosen, M. A., & Morosuk, T. (2015). Comparative exergoeconomic analyses of the integration of biomass gasification and a gas turbine power plant with and without fogging inlet cooling. *Renewable Energy*, 76, 394-400.
- Begum, S., Rasul, M., & Akbar, D. (2014). A numerical investigation of municipal solid waste gasification using Aspen Plus. *Procedia Engineering*, 90, 710-717.
- Boerrigter, H., Calis, H. P., Slort, D. J., & Bodestaff, H. (2004). Gas cleaning for integrated Biomass Gasification (BG) and Fischer-Tropsch (FT) systems; experimental demonstration of two BG-FT systems. *Acknowledgement/Preface*, 51.
- Campitelli, G., Cordiner, S., Gautam, M., Mariani, A., & Mulone, V. (2013). Biomass fueling of a SOFC by integrated gasifier: study of the effect of operating conditions on system performance. *International Journal of Hydrogen Energy*, 38(1), 320-327.
- Chen, S., Lior, N., & Xiang, W. (2015). Coal gasification integration with solid

- oxide fuel cell and chemical looping combustion for high-efficiency power generation with inherent CO₂ capture. *Applied Energy*, 146, 298-312.
- Cormos, C. C., Cormos, A. M., & Agachi, S. (2009). Power generation from coal and biomass based on integrated gasification combined cycle concept with pre-and post-combustion carbon capture methods. *Asia-Pacific Journal of Chemical Engineering*, 4(6), 870-877.
- Daigoglou, V., Wicke, B., Faaij, A. P., & Vuuren, D. P. (2015). Competing uses of biomass for energy and chemicals: Implications for long-term global CO₂ mitigation potential. *Gcb Bioenergy*, 7(6), 1321-1334.
- Digman, B., Joo, H. S., & Kim, D. S. (2009). Recent progress in gasification/pyrolysis technologies for biomass conversion to energy. *Environmental Progress & Sustainable Energy*, 28(1), 47-51.
- Dlugosel'skii, V., Belyaev, V., Mishustin, N., & Rybakov, V. (2007). Gas-turbine units for cogeneration. *Thermal Engineering*, 54(12), 1000-1003.
- dos Santos, I. F. S., Vieira, N. D. B., Barros, R. M., Filho, G. L. T., Soares, D. M., & Alves, L. V. (2016). Economic and CO₂ avoided emissions analysis of WWTP biogas recovery and its use in a small power plant in Brazil. *Sustainable Energy Technologies and Assessments*, 17, 77-84. doi:https://doi.org/10.1016/j.seta.2016.08.003
- El-Emam, R. S., Dincer, I., & Naterer, G. F. (2012). Energy and exergy analyses of an integrated SOFC and coal gasification system. *International Journal of Hydrogen Energy*, 37(2), 1689-1697.
- Gerssen-Gondelach, S., Saygin, D., Wicke, B., Patel, M. K., & Faaij, A. (2014). Competing uses of biomass: assessment and comparison of the performance of bio-based heat, power, fuels and materials. *Renewable and sustainable energy reviews*, 40, 964-998.
- Ghazizadeh, V., Ghorbani, B., Shirmohammadi, R., Mehrpooya, M., & Hamed, M. H. (2018). Advanced Exergoeconomic Analysis of C3MR, MFC and DMR Refrigeration Cycles in an Integrated Cryogenic Process. *Gas Processing*, 6(1), 41-71. doi:10.22108/gpj.2018.111251.1032
- Ghorbani, B., Shirmohammadi, R., & Mehrpooya, M. (2018). A novel energy efficient LNG/NGL recovery process using absorption and mixed refrigerant refrigeration cycles—Economic and exergy analyses. *Applied Thermal Engineering*, 132, 283-295.
- Ghorbani, B., Shirmohammadi, R., Mehrpooya, M., & Hamed, M.-H. (2018). Structural, operational and economic optimization of cryogenic natural gas plant using NSGAI two-objective genetic algorithm. *Energy*, 159, 410-428. doi:https://doi.org/10.1016/j.energy.2018.06.078
- Ghorbani, B., Shirmohammadi, R., Mehrpooya, M., & Mafi, M. (2018). Applying an integrated trigeneration incorporating hybrid energy systems for natural gas liquefaction. *Energy*, 149, 848-864.
- Guo, P., Saw, W. L., Van Eyk, P. J., Stechel, E. B., Ashman, P. J., & Nathan, G. J. (2017). System Optimization for Fischer-Tropsch Liquid Fuels Production via Solar Hybridized Dual Fluidized Bed Gasification of Solid Fuels. *Energy & Fuels*, 31(2), 2033-2043.
- Hamed, M.-H., Shirmohammadi, R., Ghorbani, B., & Sheikhi, S. (2015). Advanced Exergy Evaluation of an Integrated Separation Process with Optimized Refrigeration System. *Gas Processing*, 3(1), 1-10. doi:10.22108/gpj.2015.20181
- Hanaoka, T., Liu, Y., Matsunaga, K., Miyazawa, T., Hirata, S., & Sakanishi, K. (2010). Bench-scale production of liquid fuel from woody biomass via gasification. *Fuel Processing Technology*, 91(8), 859-865.
- Herz, G., Reichelt, E., & Jahn, M. (2017). Design and evaluation of a Fischer-Tropsch process for the production of waxes from biogas. *Energy*, 132, 370-381.

- Higman, C., & Van der Burgt, M. (2011). *Gasification*: Gulf professional publishing.
- Hlavacek, T., Zheng, L., & Furimsky, E. (1994). ASPEN Simulation of Cogeneration Plants. *CANMET Energy Technology Center Report*.
- Kaniyal, A. A., van Eyk, P. J., Nathan, G. J., Ashman, P. J., & Pincus, J. J. (2013). Polygeneration of liquid fuels and electricity by the atmospheric pressure hybrid solar gasification of coal. *Energy & Fuels*, 27(6), 3538-3555.
- Li, X., Grace, J., Watkinson, A., Lim, C., & Ergüdenler, A. (2001). Equilibrium modeling of gasification: a free energy minimization approach and its application to a circulating fluidized bed coal gasifier. *Fuel*, 80(2), 195-207.
- Li, Y.-W. (2004). *Clean diesel production from coal based syngas via Fischer-Tropsch synthesis: Technology status and demands in China*. Paper presented at the Plenary Lecture at International Pittsburgh Coal Conference.
- Mavukwana, A., Jalama, K., Ntuli, F., & Harding, K. (2013). *Simulation of sugarcane bagasse gasification using aspen plus*. Paper presented at the International Conference on Chemical and Environmental Engineering (ICCEE), Johannesburg, South Africa.
- Meratizaman, M., Monadizadeh, S., Ebrahimi, A., Akbarpour, H., & Amidpour, M. (2015). Scenario analysis of gasification process application in electrical energy-freshwater generation from heavy fuel oil, thermodynamic, economic and environmental assessment. *International Journal of Hydrogen Energy*, 40(6), 2578-2600.
- Mustafa, M. F., Nord, N., Calay, R. K., & Mustafa, M. Y. (2017). A Hybrid Biomass Hydrothermal Gasification-Solid Oxide Fuel Cell System Combined with Improved CHP Plant for Sustainable Power Generation. *Energy Procedia*, 112, 467-472.
- Pantaleo, A. M., Giarola, S., Bauen, A., & Shah, N. (2014a). Integration of biomass into urban energy systems for heat and power. Part I: An MILP based spatial optimization methodology. *Energy Conversion and Management*, 83, 347-361.
- Pantaleo, A. M., Giarola, S., Bauen, A., & Shah, N. (2014b). Integration of biomass into urban energy systems for heat and power. Part II: Sensitivity assessment of main techno-economic factors. *Energy Conversion and Management*, 83, 362-376.
- Preciado, J. E., Ortiz-Martinez, J. J., Gonzalez-Rivera, J. C., Sierra-Ramirez, R., & Gordillo, G. (2012). Simulation of synthesis gas production from steam oxygen gasification of Colombian coal using Aspen Plus®. *Energies*, 5(12), 4924-4940.
- Rafati, M., Wang, L., Dayton, D. C., Schimmel, K., Kabadi, V., & Shahbazi, A. (2017). Techno-economic analysis of production of Fischer-Tropsch liquids via biomass gasification: The effects of Fischer-Tropsch catalysts and natural gas co-feeding. *Energy Conversion and Management*, 133, 153-166.
- Salemme, L., Simeone, M., Chirone, R., & Salatino, P. (2014). Analysis of the energy efficiency of solar aided biomass gasification for pure hydrogen production. *International Journal of Hydrogen Energy*, 39(27), 14622-14632.
- Salomón, M., Gomez, M. F., & Martin, A. (2013). Technical polygeneration potential in palm oil mills in Colombia: A case study. *Sustainable Energy Technologies and Assessments*, 3, 40-52. doi:https://doi.org/10.1016/j.seta.2013.05.003.
- Sheikhi, S., Ghorbani, B., Shirmohammadi, R., & Hamed, M.-H. (2014). Thermodynamic and Economic Optimization of a Refrigeration Cycle for Separation Units in the Petrochemical Plants Using Pinch Technology and Exergy Syntheses Analysis. *Gas Processing*, 2(2), 39-51. doi:10.22108/gpj.2014.20422
- Shirmohammadi, R., Ghorbani, B., Hamed, M., Hamed, M.-H., & Romeo, L. M. (2015). Optimization of mixed refrigerant systems in low temperature applications by means of group method of data handling

- (GMDH). *Journal of Natural Gas Science and Engineering*, 26, 303-312.
- Sudiro, M., Pellizzaro, M., Bezzo, F., & Bertucco, A. (2010). Simulated moving bed technology applied to coal gasification. *Chemical Engineering Research and Design*, 88(4), 465-475.
- Svoboda, K., Pohořelý, M., Jeremiáš, M., Kameníková, P., Hartman, M., Skoblja, S., & Šyc, M. (2012). Fluidized bed gasification of coal-oil and coal-water-oil slurries by oxygen-steam and oxygen-CO₂ mixtures. *Fuel Processing Technology*, 95, 16-26.
- Wang, J.-J., Yang, K., Xu, Z.-L., & Fu, C. (2015). Energy and exergy analyses of an integrated CCHP system with biomass air gasification. *Applied Energy*, 142, 317-327.
- Xydis, G., Nanaki, E., & Koroneos, C. (2013). Exergy analysis of biogas production from a municipal solid waste landfill. *Sustainable Energy Technologies and Assessments*, 4, 20-28. doi:<http://dx.doi.org/10.1016/j.seta.2013.08.003>
- Yan, L., & He, B. (2017). On a clean power generation system with the co-gasification of biomass and coal in a quadruple fluidized bed gasifier. *Bioresource Technology*, 235, 113-121.
- Zheng, L., & Furimsky, E. (1999). *Computer models and simulations of IGCC power plants with Canadian coals*. Retrieved from
- Zheng, L., & Furimsky, E. (2003). ASPEN simulation of cogeneration plants. *Energy Conversion and Management*, 44(11), 1845-1851.

