HYDROGEN, FUEL CELL & ENERGY STORAGE

Process Modeling and Optimization of Coal Gasification for Enhanced Hydrogen and Syngas Yield in Sponge Iron Production

Mohsen Bahoosh | Eslam Kashi*

Department of Chemical Technologies, Iranian Research Organization for Science and Technology (IROST), Tehran, Iran
* Corresponding author, Email: kashi@irost.ir

Article Information

Article Type
Research Article

Article History
Received: *17 Jul 2026*
Revised: *14 Oct 2026*
Accepted: *24 Oct 2026*
Published Online: *30 Oct 2026*

Keywords

Coal gasification
Syngas
Tabas coal
Steel
Aspen Plus

Abstract

Due to the irregular availability of natural gas, coal has been proposed as an alternative source for the production of synthesis gas in steel plants. This study simulated a coal gasification unit aimed at producing synthesis gas. The developed model was initially validated using available reference data, confirming its reliability and accuracy. Using Tabas coal as feedstock, the gasification process was simulated in Aspen Plus software using an entrained-flow gasifier. Sensitivity analysis was conducted on the type of coal, as well as the water-to-coal and oxygen-to-coal ratios, to identify key factors affecting the gasification process. The key results show that approximately 22 tons per hour of Tabas coal are required to produce 77000 Nm^3/h of syngas, sufficient to support the production of 110 tons per hour of sponge iron. Process water consumption is around 0.3 times the coal input, with a cooling and quenching water-to-coal ratio of approximately 1.7, much of which is reused. Significantly, additional water is not required for the water-gas shift reaction due to syngas quenching within the gasifier. The study confirmed that the type of coal and the ratios of water-to-coal and oxygen-to-coal are critical parameters, with high-quality Tabas coal demanding lower amounts of oxygen and water for syngas production compared to lower-grade coals. This research serves as a valuable guide for improving the efficiency and productivity of coal gasification units in the steel industry. Overall, the findings indicate that using coal for synthesis gas production has great potential in meeting energy demands and enhancing productivity in the steel industry.

Cite this article: Bahoosh, M., Kashi, E. (2026). Process Modeling and Optimization of Coal Gasification for Enhanced Hydrogen and Syngas Yield in Sponge Iron Production. DOI: 10.22104/hfe.2025.7606.1358

© The Author(s). Publisher: Iranian Research Organization for Science and Technology (IROST)
DOI: 10.22104/hfe.2025.7606.1358

1 Introduction

The iron and steel industry, which plays a crucial role in stabilizing economic growth and employment, is vital to a nation's industrial and economic development. Moreover, the steel industry is one of the most energy-intensive sectors, accounting for the largest share of energy consumption across all industrial sectors. To reduce Carbon Dioxide (CO_2) emissions and address the high energy consumption in the steel industry, Direct Reduction Iron (DRI) technology has been developed and has rapidly advanced. DRI is a process that converts iron ore into sponge iron at temperatures below the melting point. This method offers several advantages, such as lower pollution, reduced energy consumption, and immunity to the limitations caused by a shortage of coking coal, compared to the traditional rotary kiln method for iron production. Furthermore, the sponge iron produced via the DRI process is characterized by low levels of impurities such as sulfur, phosphorus, silicon, and other harmful contaminants, making it an essential raw material for manufacturing high-grade steel. Various methods exist for producing sponge iron through direct reduction. For example, in India – one of the world's largest producers of DRI sponge iron – two primary DRI production methods are employed: one uses small-scale rotary kilns that rely on coal and iron ore, while the other utilizes large-scale shaft furnaces that operate with natural gas and iron oxide pellets. Since the capacity of rotary kilns is limited and cannot fully meet the requirements of steel plants, the use of natural gas has become more common. However, when the availability of natural gas is also constrained, coal gasification emerges as a suitable alternative.

Coal gasification itself encompasses various types – such as fixed-bed, fluidized-bed, and others – and all these processes rely on the partial oxidation of carbon-containing feedstocks [1–4]. Subsequent studies on the simulation of the coal gasification process have examined the units used to define the gasifier, the parameters influencing the process, and the expected results. Nayak et al. [5] used Aspen Plus to simulate coal gasification in a fluidized bed, integrating pyrolysis, combustion, and steam gasification. They found that increasing the steam-to-coal ratio lowered (Carbon Monoxide) CO and Methane (CH_4) while raising Hydrogen (H_2) and CO_2, highlighting the importance of operating conditions in gasification. Liu et al. [6] developed a simulation model for a pressurized fluidized bed gasifier with an ash agglomerator using a sequential modular method with recycle loops. Their model, which incorporated both hydrodynamic and kinetic parameters computed via the PR–BM equation, matched experimental data well and demonstrated that optimizing oxygen-to-coal and steam-to-coal ratios can control the H_2/CO ratio.

Hu et al. [7] optimized the effective syngas fraction (H_2 + CO) in an entrained-flow gasifier using the Taguchi method, Response Surface Methodology (RSM), and the Nelder–Mead algorithm. Their study showed that the oxygen-to-coal ratio is key to maintaining stable syngas composition, with pressure also playing a regulatory role. Rudra Paol et al. [8] simulated gasification of high-ash Indian coal in a fluidized bed, varying the steam-to-coal ratio and temperature while keeping the feed rate and air-to-coal ratio constant. Their results demonstrated that hydrogen production increases with steam-to-coal ratio up to a certain temperature, whereas CO, CH_4, and CO_2 respond differently to changes in temperature and steam-to-coal ratio, affecting overall carbon conversion. Dang et al. [8] simulated Shenmu coal gasification by dividing the process into pyrolysis and gasification stages. Their model, which included preheating, mixing, heat exchange, separation, and cooling (with both direct and indirect heat transfer), showed that higher water-to-coal ratios at lower temperatures boost hydrogen production and reduce CO and CO_2, with a novel quench loop improving water recycling and process stability. Zhang et al. [9] created a five-unit thermodynamic equilibrium model for Synthetic Natural Gas (SNG) production from coal gasification in Aspen Plus (V10), considering both dry and slurry feed as well as bituminous and lignite coals. Sensitivity analysis revealed that the O_2/coal ratio is critical – an optimal value of 0.6 yields high-quality SNG – while CO_2 flow and water-to-coal ratios also significantly influence the higher heating value and overall gas quality. Shahabuddin et al. [10] simulated coal gasification using various reactants to maximize hydrogen yield, validating their model against experimental data. They found that steam-O_2 reactants provided the highest H_2/CO ratio (0.74), and catalytic water-gas shift reaction (WGSR) at 400 °C (steam/coal ratio 1.2) ensured complete CO conversion for optimal H_2.

Zhou et al. [11] simulated and optimized a two-stage pulverized coal gasification process in Aspen Plus for hydrogen-rich production, studying gasification pressure, steam-coal ratio (SCR), and oxygen-coal ratio (OCR). They identified optimal conditions (SCR 0.3, OCR 0.53) yielding 77.78 g/kg coal H_2, 48.38% higher than single-stage gasification. Saufishan et al. [12] developed a kinetic model in Aspen Plus for corn stover gasification to optimize hydrogen production. Their findings indicated that steam gasification achieved a maximum hydrogen production efficiency (HPE) of 59%, superior to air gasification (26%), with an optimal gasifying agent flow rate of 1200 kg/h

at 900 °C. Yinan et al. [13] developed a thermodynamic model of a Shell entrained flow coal gasifier in Aspen Plus for Integrated Gasification Combined Cycle plants (IGCC) power plants, validating it against published data. Their analysis showed that the oxygen-to-coal ratio is the most significant parameter (optimal ≈ 0.85), while the water-to-coal ratio critically influences hydrogen concentration and syngas composition based on energy availability. J. Zhang et al. [14] modeled a dual-fluidized bed biomass gasification process in Aspen Plus to investigate operational control characteristics and parameter influence. They found that fuel feed rate and circulating bed material correlated positively with gas heat value, carbon conversion, and efficiency, while air equivalent ratio and steam/biomass ratio showed varied effects on gas production rate, carbon conversion, and gas heat value.

Y. Zhang et al. [15] developed a kinetic-free thermodynamic model in Aspen Plus for SNG production via coal gasification in an entrained flow gasifier, validated against empirical data. They identified the O_2/coal ratio as a key factor (optimal 0.2-0.6 for Coal gas efficiency (CGE)), finding that increasing CO_2 flow improved syngas Higher Heating Value (HHV), while increasing the water-to-coal ratio decreased HHV.

Notably, all these studies employ several reactors and separators to define the gasifier, due to the absence of a dedicated gasifier process unit in the Aspen software. Consequently, in simulating the unit, various processes occurring throughout the gasifier (such as dehydration, pyrolysis, gasification, separation of volatile materials, etc.) are simulated using different equipment. While recent studies have significantly advanced coal and biomass gasification modeling- exploring various reactor configurations, kinetic mechanisms, and optimization strategies for specific products like hydrogen or SNG- a critical research gap persists in the comprehensive and integrated simulation of the entire coal-to-synthesis gas process specifically designed and optimized for direct application within steel plants. Existing simulations often focus on isolated gasifier units, employ generic coal types, or target different end products, overlooking the specific insights crucial for optimizing industrial processes that rely on particular local feedstocks, such as Tabas coal. Furthermore, despite advancements, a detailed and integrated modeling of crucial downstream processes, especially rapid syngas quenching for accurate process water management, has not been fully presented within such comprehensive steel-plant oriented simulations. Addressing this gap is of paramount importance for the steel industry, particularly in regions facing fluctuating natural gas supplies, as it enables the optimized utilization of indigenous coal resources like Tabas coal, leading to enhanced energy efficiency, reduced operational costs, and a more sustainable domestic supply of synthesis gas for sponge iron production.

In this study, for the first time, all the operational units required for converting coal into synthesis gas for a steel plant have been simulated using Aspen Plus V14. Moreover, unlike previous research, the rapid quenching process in the gasifier has been fully modeled to allow for a more precise calculation of the process water requirement.

2 Material and Methods

2.1 Base simulation

In this section, the initial simulation was performed as a reference and compared with experimental data and other models to verify the simulation approach and input data. The simulation describes a Gibbs free energy-based model for Texaco entrained-flow gasifiers and follows the modeling approach proposed by Wen and Chang [16, 17]. The key features of the model include:

- Steady-State Operation: The model is carried out under steady-state conditions.
- Comprehensive Process Representation: It captures the main physical and chemical processes within the gasifier, including coal pyrolysis, volatile combustion, and coke gasification.
- Instantaneous Mixing: It is assumed that the gaseous phase is instantly and completely mixed with the solid phase.
- Negligible Pressure Drop: The pressure drop in the gasifier is disregarded.

2.1.1 Material specifications

During the gasification process, various materials and compounds are produced. This section presents their corresponding chemical components (Table 1).

2.1.2 Pilot gasifier process description

The pilot gasifier, whose data is used to evaluate the simulation in this project, is briefly reviewed here. The Texaco gasifier is an entrained-flow design. This steel vessel – with a diameter of 5.1 meters and a length of 1.6 meters – is internally divided into two sections. The upper section is lined with a special refractory material designed to withstand harsh operating conditions and is dedicated to coal gasification. In this process, powdered coal (with particle sizes smaller than 500 μm) is mixed with water to form a coal-water slurry, which, together with oxygen, is fed into the upper section.

Table 1. Chemical Components Used in the Model [16, 17].

ID	Type	Name	Formula
O_2	Conv	Oxygen	O_2
CO	Conv	Carbon-Monoxide	CO
H_2	Conv	Hydrogen	H_2
CO_2	Conv	Carbon-Dioxide	CO_2
H_2O	Conv	Water	H_2O
H_2S	Conv	Hydrogen-Sulfide	H_2S
N_2	Conv	Nitrogen	N_2
CH_4	Conv	Methane	CH_4
C_6H_6*	Conv	Benzene	C_6H_6
C	Solid	Carbon-Graphite	C
S	Solid	Sulfur	S
COAL	NC	–	–
CHAR1*	NC	–	–
CHAR2*	NC	–	–
ASH	NC	–	–

Here, coal pyrolysis, volatile combustion, and coke gasification occur to produce synthesis gas under operating pressures of 20-50 atmospheres and temperatures exceeding 1000 °C [16, 17]. The lower section serves as a cooling chamber. A water reservoir continuously supplies cooling water at the bottom, where ash and synthesis gas exit from the upper section. The ash remains in the water and is later removed, while the saturated synthesis gas is drawn from above the water. Although commercial petroleum-based gasifiers are designed to operate at pressures up to 80 atmospheres, the coal-based pilot unit is designed for a maximum pressure of 28 atmospheres [18].

2.1.3 Physical properties and feed specifications

In this project, the Redlich-Kwong-Soave (RK-SOAVE) method is used to calculate the physical properties of conventional mixture components as well as Conventional Insoluble Solid (CISOLID) components. To evaluate the unconventional components, the Enthalpy Coal Generate (HCOALGEN) and Density Coal Ignore Trace (DCOALIGT) models are employed for determining enthalpy and density, respectively. The HCOALGEN model requires three key analyses for the unconventional components:

- Proximate Analysis (PROXANAL): Provides the weight fractions of moisture, fixed carbon, volatile matter, and ash.
- Ultimate Analysis (ULTANAL): Gives the weight percentages of ash, carbon, hydrogen, nitrogen, chlorine, sulfur, and oxygen.
- Sulfur Analysis (SULFANAL): Breaks down the sulfur content into pyritic, sulfate, and organic sulfur fractions.

Table 2 presents the characteristics of the coal component used in the base model, adopted from the modeling work of Wen and Chuang [16, 17]. Based on these specifications, the coal's enthalpy and density are calculated. The same procedure is applied to the char and ash produced during coal conversion; their enthalpy and density are determined using the same models, with analysis results obtained from a mass balance based on the original coal analysis data and the amount of gasified product. Since Aspen Plus does not offer a dedicated graphical block for a gasifier, several reactors are used for the simulation. For example, when coal enters the gasifier, it first undergoes pyrolysis to convert into volatile products and char. The corresponding chemical reaction is shown in Equation (1):

$$\text{Coal} \longrightarrow \text{Char} + \text{CO} + \text{H}_2 + \text{H}_2\text{O} + \text{CO}_2 + \text{CH}_4 + \text{H}_2\text{S} + \text{N}_2 + \text{C}_6\text{H}_6 \quad (1)$$

Table 2. Feed Coal Specifications [16, 17]

Proximate analysis		Ultimate analysis		Sulfur analysis	
Element	Value (wt.%)	Element	Value (wt.%, dry basis)	Element	Value (wt.%, dry basis)
Moisture (wet basis)	0.2	C	74.05	Pyritic	0.59
Fixed carbon (dry basis)	58.01	H	6.25	Sulfate	0.59
Volatile matter (dry basis)	26.46	N	0.71	Organic	0.59
Ash (dry basis)	15.53	Cl	0.37		
		S	1.77		
		O	1.32		
		Ash	15.53		

In the presented model, the volatile components include CO, H_2, Water (H_2O), CO_2, CH_4, Hydrogen Sulfide (H_2S), Nitrogen (N_2), and Benzene (C_6H_6). A separate reactor is designated for these reactions, and the yield of coal conversion into char and volatiles is presented in Table 3 based on laboratory results by

Wen and Chuang. For a more precise outcome, Equation (2) can be employed and the conversion yield adjusted according to the reactor's operating pressure (24 atm) [16, 17].

$$V_2 = V_1(1 - \alpha \ln P_t) \tag{2}$$

where V_1 is total yield of volatiles at 1 atm, V_2 is total yield of volatiles at the pressure of the real gasifier, P_t is pressure in real gasifier (atm.), and α is a constant. In this model, $\alpha = 0.066$.

Table 3. Coal Conversion Yield to Char and Volatiles at 1 atm [16, 17].

Components	Yield (mass basis on original coal)
CO	0.0059
H_2	0.0084
CO_2	0.003
H_2O	0.0079
H_2S	0.0094
N_2	0.0035
CH_4	0.1637
C_6H_6	0.071
Char	0.7272
Total	1

2.1.4 Unit flow sheet

Figure 1 presents the overall flow of the coal gasification process. In this model, the cooling section for the hot gas is not simulated. The function of each block is detailed in Table 4, while additional feed specifications are provided in Table 5. Blocks B1 and B2 are used for simulating coal pyrolysis, Block B3 models the volatile combustion process, and Block B7 is dedicated to coke gasification. The remaining blocks assist in simulating these three main processes. As shown in Table 5, the coal is preheated to a temperature range of 100-300 °C, which facilitates easier transfer and improves gasification efficiency [16, 17].

2.1.5 Examination of the base simulation results

Based on the input conditions provided in the previous section, the gasifier output results were obtained and are presented in Table 6 as part of the Aspen Plus model. For comparison, the results from Wen and Chaung's work are also shown in the table. It is evident that Wen and Chaung's results more closely match the experimental data. In the base simulation, the CO flow rate and carbon conversion are slightly higher than the experimental values, while the CO_2 flow rate is somewhat lower.

Table 4. Explanation of the Base Simulation Blocks

Block	Model	Function
B1	RYield	Simulation of coal pyrolysis based on pyrolysis test results at 1 atm pressure.
B2	RYield	Adjustment of each product's yield from the pyrolysis test pressure (i.e., 1 atm) to the actual gasifier pressure.
B3	RStoic	Stoichiometric modeling of volatile gas combustion.
B4	Sep2	Separation of gases and char.
B5	RStoic	Conversion of char into C, H_2, O_2, N_2, S, and ash.
B6	Mixer	Mixing of the feed and steam.
B7	RGibs	Gasification of the feed mixture.

The discrepancies in the CO and CO_2 flow rates and carbon conversion may stem from several factors: the use of Gibbs free energy instead of stoichiometric relations, the lack of direct consideration of reactor dimensions and residence time, and the higher gasifier outlet temperature calculated by base model. In the presented model, the outlet temperature is 1766 K compared to around 1422 K in the Wen and Chaung model. The higher temperature accelerates the reactions between solid carbon and gases (i.e., Equations (3) to (6)), resulting in a higher carbon conversion than observed experimentally. Additionally, differences in the CO and CO_2 flow rates are linked to Equation (7), an exothermic reaction. A temperature increase causes this reaction to shift in the reverse direction – leading to a higher production of CO and a lower production of CO_2. Consequently, the elevated temperature reduces the simulated CO_2 flow rate while increasing the simulated CO flow rate.

$$\mathrm{C} + \frac{1}{\varphi}\mathrm{O_2} \longrightarrow 2\left(1 - \frac{1}{\varphi}\right)\mathrm{CO} + \left(\frac{2}{\varphi} - 1\right)\mathrm{CO_2} \tag{3}$$

$$\mathrm{C} + \mathrm{H_2O} \longrightarrow \mathrm{CO} + \mathrm{H_2} \tag{4}$$

$$\mathrm{C} + \mathrm{CO_2} \longrightarrow 2\,\mathrm{CO} \tag{5}$$

$$\mathrm{C} + 2\,\mathrm{H_2} \longrightarrow \mathrm{CH_4} \tag{6}$$

$$\mathrm{CO} + \mathrm{H_2O} \longrightarrow \mathrm{CO_2} + \mathrm{H_2} \tag{7}$$

φ is a coefficient that depends on the diameter of coal particles. There are two reasons why the base simulation results in a higher gasifier temperature. The first reason is the coal combustion heat (HCOMB). In the base model, the HCOMB of the coal is calculated using the Boie correlation in Aspen Plus due to the lack of precise experimental data. However, HCOMB has a significant impact on the coal's enthalpy; an inaccurate value for HCOMB may lead to an incorrect coal enthalpy, and consequently, a substantial deviation in the gasifier temperature. The second reason

is the amount of heat loss in the gasifier. In the base simulation, the model is simulated under adiabatic conditions, whereas in Wen and Chaung's model, heat loss to the environment is considered. Therefore, the combination of these two factors may result in a higher gasifier temperature in the base model.

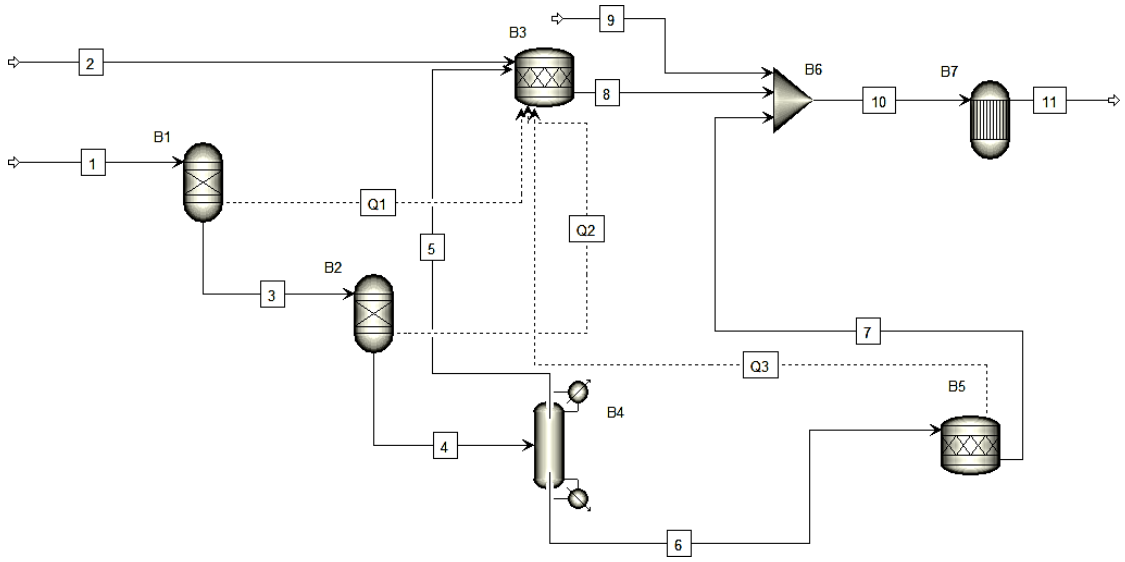

Fig. 1. Base Simulation Flow Sheet.

Table 5. Specifications of Feed Streams in the Base Simulation

Feedstock	Stream ID	Parameter	Value	Unit
Coal	1	Flow rate	76.66	g/s
		Temperature	505.22	K
		Pressure	24	atm
		Diameter of particle	350	μm
		Velocity entering into gasifier	3	m/s
Oxygen	2	Ratio of oxygen to coal flow rates	0.866	dimensionless
		Temperature	298	K
		Pressure	24	atm
Steam	9	Ratio of steam to coal flow rates	0.241	dimensionless
		Temperature	696.67	K
		Pressure	24	atm

Table 6. Comparison of Base Simulation Results, Experimental Data, and Wen & Chang's Model [8, 9].

	Experimental		Wen and Chaung's model		Aspen Plus model a		Aspen Plus model b	
Parameters	Flow rate (g/s)	Mole fraction (%, dry basis)	Flow rate (g/s)	Mole fraction (%, dry basis)	Flow rate (g/s)	Mole fraction (%, dry basis)	Flow rate (g/s)	Mole fraction (%, dry basis)
CO	123.77	57.57	123.94	56.60	127.7	58.69	124.57	57.55
H_2	6.01	39.13	6.23	39.84	6.02	38.48	5.94	38.16
CO_2	9.985	2.95	10.04	2.92	6.92	2.02	10.16	2.98
CH_4	0.15	0.12	0.20	0.16	0.013	0.010	0.62	0.499
H_2S	0.133	0.06	0.726	0.27	1.44	0.54	1.44	0.54
N_2	0.53	0.12	0.454	0.208	0.54	0.25	0.54	0.25
Carbon conv. (%)	98.64		98.88		100		100	
Temp. (K)	–		1421.9		1766.25		1416.47	

**In model a, HCOMB is calculated using the Boie correlation; whereas in model b, the coal HCOMB is manually set to 13,416 Btu/lb.

To further investigate the above explanation – which leads to differences in the CO and CO_2 flow rates and carbon conversion due to the higher temperature in the base model – in case b, HCOMB for the coal is manually entered so that the gasifier outlet temperature from the base simulation matches that of Wen and Chaung's work.

When HCOMB is manually set to 13,416 Btu/lb (compared to the coal HCOMB calculated as 83/14080 Btu/lb using the Boie correlation), the gasifier outlet temperature becomes 1416 K, which is in good agreement with the 1422 K reported in Wen and Chaung's work. Under these conditions, the flow rates of CO and CO_2 also closely match the experimental data. These observations indicate that the product gas composition and carbon conversion are highly dependent on the gasifier temperature, and that both the coal HCOMB and heat loss are key parameters in determining the gasifier temperature.

2.2 Simulation of the gasification unit

In this section, based on the model derived from the base simulation and incorporating information from other studies, first, some existing issues are examined before the simulation of the gasification unit is carried out.

2.2.1 Feed specifications for Tabas Coal

Comparison of the analysis results presented in various studies [19–21] shows that coal analysis can vary depending on the location, stratum, and sampling conditions. For instance, the moisture content reported in the study by Talakoub and Rajabzadeh is about 1%, whereas in the report by Rāyegān and Eskandari it is 9%. Considering the more comprehensive report by Rajabzadeh et al. [20] an adjusted average of the data from this report has been used as the reference analysis for the simulation, as shown in Table 7.

Table 7. Proximate and Ultimate Analysis of Tabas Anthracite Coal According to Rajabzadeh et al. [17].

Proximate analysis (% by wt)				Ultimate analysis (% by wt)					Forms of sulfur		
FC (d)	M (ad)	V (daf)	A (d)	O (daf)	H (daf)	N (daf)	C (daf)	St (d)	Sp (d)	Ss (d)	So (d)
54.075	0.8	22.475	23.45	6.34	15.8	7.38	64.64	5.84	4.46	0.17	1.21

** FC, fixed carbon, M, moisture; VM, volatile matter; Ash, ash yield; O, Oxygen H, hydrogen; N, nitrogen; C, carbon; St, total sulfur; Sp, pyritic sulfur; Ss, sulfatic sulfur; So, organic sulfur; ad, air-dry basis; d, dry basis; daf, dry and ash-free basis.

Table 8. The specifications of Tabas coal, which serve as the input data for the software.

Proximate analysis		Ultimate analysis		Sulfur analysis	
Element	Value (wt.%)	Element	Value (wt.%, dry basis)	Element	Value (wt.%, dry basis)
Moisture	0.8	Ash	23.45	Pyritic	3.41
Fixed carbon (dry basis)	54.075	Carbon	49.48	Sulfate	0.14
Volatile matter(dry basis)	22.475	Hydrogen	12.1	Organic	0.92
Ash (dry basis)	23.45	Nitrogen	5.65		
		Chlorine	0		
		Sulfur	4.47		
		Oxygen	4.85		

The specifications of Tabas coal, which serve as the input data for the software, are ultimately presented in Table 8.

2.2.2 Simulation assumptions

In this simulation, the following assumptions have been applied: The process is carried out under steady-state conditions. Ash is considered an inert material with no catalytic activity and does not participate in the gasification process. Both heat and pressure losses are neglected. All reactions are assumed to reach equilibrium, and reaction kinetics are not taken into account. Drying and pyrolysis occur simultaneously, with the volatile products consisting of H_2, CO, CO_2, CH_4, and H_2O. The operating conditions are based on an Entrained Flow gasifier (with a pressure range of 20 to 50 atmospheres and temperatures above 1000 °C). In this model, the RK-SOAVE method is used to calculate the physical properties of conventional components and CISOLID components, while the HCOALGEN and DCOALIGT models are used to calculate the enthalpy and density of the unconventional components, respectively. Since Aspen Plus does not provide a dedicated

graphical block for a gasifier unit, several different reactors are used to simulate the gasifier. The air separation unit and feed preparation unit are not simulated; instead, oxygen and coal are directly fed into the gasifier in this modeling. The reactions occurring in the gasifier are as follows [22]:

$$C + O_2 \longrightarrow CO_2 \tag{8}$$

$$C + \frac{1}{2}O_2 \longrightarrow CO \tag{9}$$

$$H_2 + \frac{1}{2}O_2 \longrightarrow H_2O \tag{10}$$

$$C + H_2O \longrightarrow CO + H_2 \tag{11}$$

$$C + 2\,H_2O \longrightarrow CO_2 + 2\,H_2 \tag{12}$$

$$C + CO_2 \longrightarrow 2\,CO \tag{13}$$

$$C + 2\,H_2 \longrightarrow CH_4 \tag{14}$$

$$CO + H_2O \longrightarrow CO_2 + H_2 \tag{15}$$

$$CO + 3\,H_2 \longrightarrow CH_4 + H_2O \tag{16}$$

$$C + H_2O \longrightarrow \frac{1}{2}CH_4 + \frac{1}{2}CO_2 \tag{17}$$

Most of the oxygen injected into the gasifier is consumed in reactions (8) to (10) to supply the required heat for drying the fuel, breaking chemical bonds, and raising the reactor temperature to achieve the gasification reactions (reactions (11) to (17)). An oxygen-to-coal ratio of 0.8 and a steam-to-coal ratio of 0.3 have been considered [23, 24]. The total coal feed is calculated based on the process flow diagram (PFD) of the Ghaenat Steel Complex in South Khorasan and is designed for an inlet synthesis gas flow rate of approximately 77000 Nm^3/hr to the DRI furnace for the production of 110 tons per hour of sponge iron.

2.3 Operational units

This section thoroughly examines the essential operational units required in the post-gasification process. These units include the Water-Gas Shift Unit, crucial for adjusting the hydrogen to carbon monoxide ratio; the Acid Gas Separation Unit, which removes undesirable compounds like hydrogen sulfide and carbon dioxide; the Dehydration Unit, responsible for extracting moisture from the syngas; and finally, the Pressure Regulation Unit, which prepares the syngas for subsequent applications.

Water-gas shift unit. The synthesis gas produced in the gasifier must be reprocessed before it can be utilized in downstream units. WGSR is employed to adjust the chemical composition of the synthesis gas and increase the hydrogen to carbon monoxide ratio. In fact, the water-gas shift reaction is a vital step in coal gasification, where the synthesis gas is passed over a fixed-bed reactor containing shift catalysts, converting CO and H_2O into CO_2 and H_2 [25]:

$$CO + H_2O \longrightarrow CO_2 + H_2 \tag{18}$$

This reaction is typically catalyzed by various materials depending on the operating temperature [26–28].

High-temperature synthesis gas from the gasifier can be processed in one of two ways:

- *Direct water quenching*: The gas is rapidly cooled through direct water contact, saturating it with steam and eliminating the need for additional steam in the water-gas shift reaction. This method is commonly used in hydrogen and ammonia production facilities [18].
- *Gas cooling via a gas cooler*: The gas is cooled using a gas cooler, which generates a separate high-pressure steam stream.

Furthermore, the water-gas shift (WGS) reactor can be placed either before sulfur removal (acid shift) or after it (sweet shift). In the acid shift, operating at 232-260 °C with a cobalt-molybdenum catalyst, the water-saturated gas converts CO and H_2O into CO_2 and H_2 while also transforming COS into H_2S, thus easing subsequent sulfur removal. Although the sweet shift can operate at higher temperatures (HT: 288-482 °C) with iron-based catalysts or at lower temperatures (LT: 204-260 °C) with copper-zinc-alumina catalysts, it often demands additional steam injection. For coal gasification, the acid shift is generally preferred because the moisture recovered from the water scrubber effectively drives the reaction to achieve the desired H_2/CO ratio [1].

Acid gas separation. Acid gas separation units using amine gas treating are employed to remove acid gases, such as H_2S and CO_2, from gas streams (e.g., natural gas or synthesis gas). This process operates on the principle of chemically absorbing the acid gases into amine solutions [29–32]. In Iran, companies like SAZEH, PIDEK, ODCC, and EIED are active in constructing petrochemical facilities, while the domestic technology and capability now exist to build both water-gas shift and acid gas separation units.

Dehydration unit. The dehydration unit in the coal gasification process plays a critical role in removing moisture and water vapor from the synthesis gas (syngas) exiting the gasifier reactor (Table 9). This operation is essential to prevent problems such as corrosion, gas hydrate formation, and disruptions in downstream processes (e.g., chemical synthesis or combustion). Triethylene glycol (TEG) is the most commonly used glycol for syngas dehydration due to its non-corrosive

properties, high boiling point, anti-foaming characteristics, low vapor pressure, low cost, and the ability to regenerate up to 98% [33–37]. In this project, based on the process requirements, the glycol dehydration method was selected.

Pressure regulation unit. To reduce the pressure of the synthesis gas stream from 24 bar to 1.5 bar, several technical options are available. These options differ in terms of installation cost, maintenance cost, energy efficiency, and operational considerations. A comparative outlining these options is provided in Table 10. Based on the considerations outlined in table, an expander turbine will be used in this project for regulating the pressure of the synthesis gas.

Table 9. Comparison of Dehydration Methods [33–37].

Parameter	Glycol (TEG)	Molecular Sieve	Condensation
Moisture output	$\approx 0.1\%$ volume	$\approx 0.001\%$ volume	$\approx 5\%$ volume
Capital cost	Medium	High	Low
Energy consumption	Medium (reboiler)	High (high-temp regen)	Low (cooling only)
Application	Natural gas/Syngas	Petrochemical Industry	Pre-treatment

Table 10. Overall Comparison of Pressure Regulation Methods

Option	Installation Cost	Maintenance Cost	Energy Efficiency	Recommended Application
PRV (Pressure Relief Valve)	Low	Low	Low	Low-capacity systems / Budget-limited setups
Expander turbine	Very high	High	Very high	High-capacity systems / Energy recovery needs
Flow control valve	Very low	Very low	Very low	Temporary / Emergency pressure reduction
Multi-stage system	Medium	Medium	Medium	Pressure reduction with minimal noise/vibration

3 Results and Discussion

The blocks in the simulated PFD of the gasification unit are depicted in Figure 2. The corresponding block naming conventions are provided in Table 11, while the simulation results are presented in Table 13 (See supplementary).

3.1 Sensitivity analysis

This section presents a sensitivity analysis of critical parameters influencing the gasification process. Specifically, the analysis investigates the impact of the Oxygen-to-Coal and Water-to-Coal Ratios, as well as the Effect of Coal Type, on the overall gasification performance and syngas characteristics.

3.1.1 Oxygen-to-Coal and Water-to-Coal ratios

As discussed in the literature review, the H_2/CO ratio in the syngas produced from coal gasification is influenced by several factors, including the O_2/Coal and Water/Coal ratios:

- O_2*/Coal ratio*: Increasing the oxygen-to-coal ratio typically results in greater production of CO and H_2. However, the CO increase is generally more significant, which may reduce the H_2/CO ratio [38].
- *Water/Coal ratio*: Raising the water-to-coal ratio enhances the water-gas shift reaction, producing more hydrogen. This leads to an increased H_2/CO ratio, as more hydrogen is generated relative to carbon monoxide [39, 40].

The effect of increased oxygen input is illustrated in Figure 3, while the impact of increased water input on the H_2/CO ratio in the gasifier outlet stream is shown in Figure 4. Variations in these parameters alter the H_2/CO ratio, and the results align with previous research findings [38–40].

3.1.2 Effect of coal type

The type and quality of coal, as the primary feedstock in the process, have a significant impact on the amount of water required to achieve the desired H_2/CO ratio. For instance, a simulation has been conducted based on the coal used in the Lurgi project and Jindal company [25] (Table 12, Figure 5).

Table 11. Specifications of simulation blocks

Block	Model	Function
B1	RYield	Simulates coal pyrolysis
B2	Sep2	Separates ash from other pyrolysis products
B3	Mixer	Mixes feed, steam, and oxygen
B4	RGibs	Gasifies the feed mixture
B5	Mixer	Combines raw syngas and water to achieve 200 °C (quench simulation)
B6	RStoic	Water-gas shift unit to adjust the H_2/CO ratio
B7	Cooler	Heat exchanger to reduce temperature to 50 °C
B8	Sep	Separates syngas and liquids
B9	Sep	Removes acid gases in the amine tower
B10	Sep	Dehydrates syngas by removing moisture.
B11	Heater	Raises syngas temperature before entering the pressure regulation unit to prevent condensation.
B12	Turbine	Regulates syngas pressure.
B13	Heater	Adjusts syngas temperature.

Table 12. Analysis of Indian Coal in the Lurgi Project and Jindal Company [25].

Element	PROXANAL	ULTANAL	SULFANAL
Moisture	7	-	-
FC	34.4	-	-
VM	27.96	-	-
Ash	37.63	37.63	-
Carbon	-	48.02	-
Hydrogen	-	3.12	-
Nitrogen	-	0.94	-
Chlorine	-	0	-
Sulfur	-	0.62	-
Oxygen	-	9.67	-
Pyritic	-	-	0.62
Sulfate	-	-	0
Organic	-	-	0

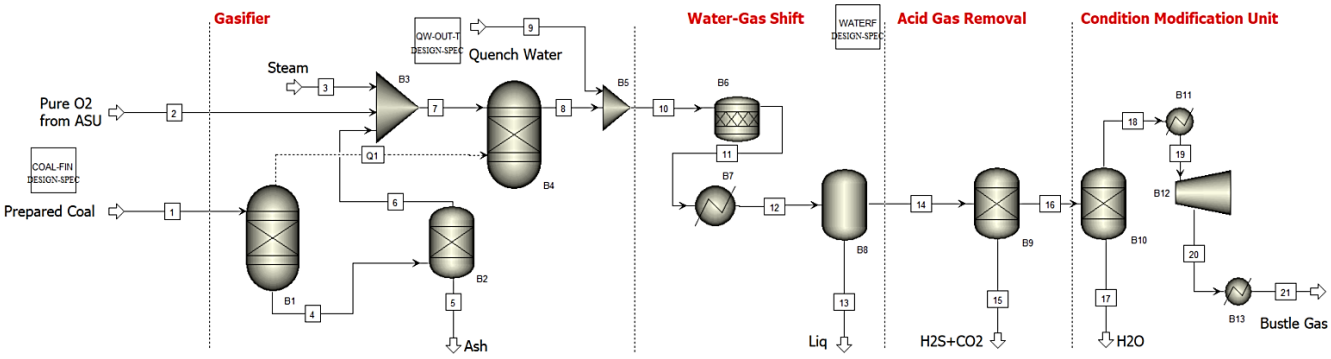

Fig. 2. PFD of the Gasification Unit.

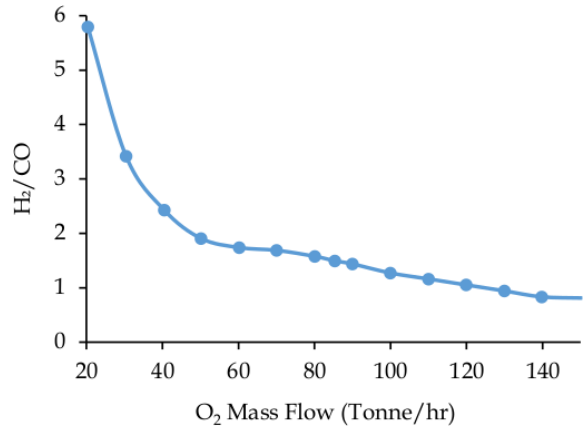

Fig. 3. Effect of Increased Oxygen Input on the H_2/CO Ratio in the Gasifier Outlet.

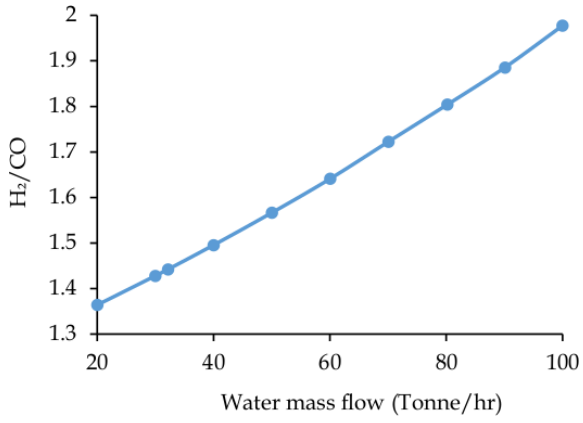

Fig. 4. Effect of Increased Water Input on the H_2/CO Ratio in the Gasifier Outlet.

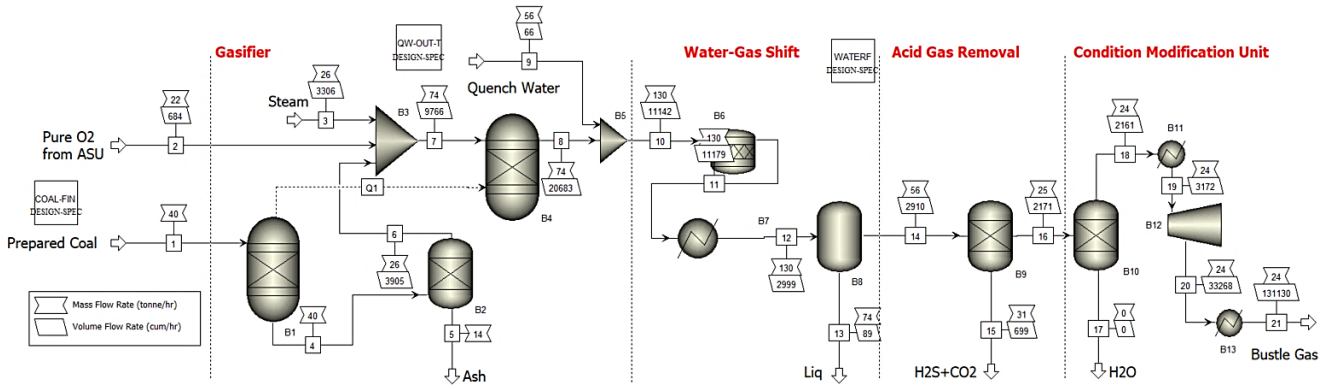

Fig. 5. PFD of the Indian Coal Gasification Unit (This process flow diagram (PFD) illustrates the Indian coal gasification unit, including mass flow rates (tons/hour), temperatures, and volumetric flow rates.)

The simulation results indicate that, assuming similar conditions at the gasifier outlet to meet volumetric and operational requirements (temperature of 839 °C and pressure of 1.4 kg/cm^2 gauge) for Ghaenat Steel Complex South Khorasan PFD, approximately 40 tons per hour of Indian coal are required. This amount is roughly double the quantity of Tabas coal needed to achieve similar conditions.

It is essential to note that comparing two systems solely by changing the type of coal is not sufficient. For a stable process (particularly in terms of temperature in the gasifier), other parameters, such as the steam-to-coal and oxygen-to-coal ratios, must also be adjusted. It should be noted that, apart from the type of gasifier, the quality of the input coal significantly influences the amounts of water and oxygen required. Lower-quality coals generally demand higher quantities of both water and oxygen [41, 42]. Consequently, the use of lower-quality coal leads to an increase in water consumption.

3.2 Limitations

It is important to acknowledge certain limitations of the current study to provide a complete context for the presented results. Firstly, the simulation is based on thermodynamic equilibrium assumptions, meaning kinetic effects are not fully considered, which may lead to deviations from real-world dynamic behavior. Secondly, for simplification, ideal mixing conditions and negligible heat and pressure losses within the gasifier and downstream units were assumed, potentially influencing the accuracy of energy balance and temperature predictions. Thirdly, while the model was rigorously validated against a comprehensive reference study, experimental data specifically from pilot-scale Tabas coal gasification under the exact modeled conditions were not available for direct comparison. Lastly, this study primarily focuses on the process modeling and optimization of syngas yields, without incorporating detailed economic analysis or a comprehensive environmental impact assessment, which are crucial considerations for full industrial feasibility.

4 Conclusions

This study successfully simulated the complete coal gasification unit required for syngas production at the Ghaenat Steel Complex in South Khorasan using Aspen Plus V14 software. The findings demonstrated that approximately 22 tons per hour of coal is required under the operational conditions (839 °C and 1.4kg/cm^2 gauge pressure) to produce 77000 Nm^3/h (131130 m^3/h in the operational conditions) of syngas for the DRI furnace, which in turn results in the production of 110 tons/hour of sponge iron. Process water consumption in the gasifier is around 0.3 times the coal input, excluding utility and auxiliary water. For cooling and quenching syngas, the water-to-coal ratio is approximately 1.7, with most of this water being treated and reused within the system. Notably, additional water input is not required for the water-gas shift reaction due to syngas quenching in the gasifier. Finally, the study concluded that high-quality Tabas coal demands lower amounts of oxygen and water for syngas production compared to lower-grade coals, making it a more efficient feedstock.

Acknowledgments

This research was conducted with the financial support of the National Steel Company and in collaboration with the management and experts of its production, localization, and research unit. The valuable contri-

butions of all involved are hereby acknowledged and appreciated.

References

[1] Gasifipedia. The National Energy Technology Laboratory (NETL) of USA;. Https://netl.doe.gov/carbonmanagement/energy-systems/gasification/gasifipedia.

[2] Hasanbeigi A. Emerging energy-efficiency and carbon dioxide emissions-reduction technologies for the iron and steel industry; 2013.

[3] Farzaneh F, Golmohammad M. Iranian hydrogen production insight: research trends and outlook. Hydrogen, Fuel Cell & Energy Storage. 2021;8(1):23-33.

[4] Ozgoli HA, Ghadamian H. Energy price analysis of a biomass gasification-solid oxide fuel cell-gas turbine power plant. Hydrogen, Fuel Cell & Energy Storage. 2016;3(1):45-58.

[5] Nayak R, Mewada RK. Simulation of coal gasification process using ASPEN PLUS. Institute of Technology; 2011.

[6] Liu Z, Fang Y, Deng S, Huang J, Zhao J, Cheng Z. Simulation of pressurized ash agglomerating fluidized bed gasifier using ASPEN PLUS. Energy & fuels. 2012;26(2):1237-45.

[7] Hou J, Zhang J. Robust optimization of the efficient syngas fractions in entrained flow coal gasification using Taguchi method and response surface methodology. International Journal of Hydrogen Energy. 2017;42(8):4908-21.

[8] Dong K, Rong Q, Li M, Lin J, Xiao R, Li Y. A novel simulation for gasification of Shenmu Coal in an entrained flow gasifier. Chemical Engineering Research and Design. 2020;160:454-64.

[9] Zhang Y, Takyi SA, Chen Q. Coal conversion to SNG: thermochemical insights through kinetic-free modeling in entrained flow gasifier. Case Studies in Thermal Engineering. 2024;56:104266.

[10] Shahabuddin M, Bhattacharya S. Process modelling for the production of hydrogen-rich gas from gasification of coal using oxygen, CO2 and steam reactants. International Journal of Hydrogen Energy. 2021;46(47):24051-9.

[11] Zhou B, Chang J, Li J, Hong J, Wang T, Zhu Z, et al. Two-stage gasification process simulation and optimization of pulverized coal for hydrogen-rich production using Aspen plus. International Journal of Hydrogen Energy. 2024;49:849-60.

[12] TA S, Rafey A, Siddiqui FZ. Hydrogen production via gasification of corn stover: modeling and simulation using Aspen Plus®. Biofuels. 2024;15(6):723-33.

[13] Yinan W, Jiayang L, Heng C, Guoqiang ZHANG GX, Rongrong Z. Research on Modeling and Variable Operating Condition Characteristics of Entrained Flow Coal Gasifier Based on Aspen Plus. Power Generation Technology. 2024;45(5):951.

[14] Zhang J, Yang L. Aspen simulation study of dual-fluidized bed biomass gasification. Energies. 2024;17(10):2381.

[15] Zhang Y, Takyi SA, Chen Q. Coal conversion to SNG: thermochemical insights through kinetic-free modeling in entrained flow gasifier. Case Studies in Thermal Engineering. 2024;56:104266.

[16] Wen CY, Chaung T. Entrainment coal gasification modeling. Industrial & Engineering Chemistry Process Design and Development. 1979;18(4):684-95.

[17] Wen C. Noncatalytic heterogeneous solid-fluid reaction models. Industrial & Engineering Chemistry. 1968;60(9):34-54.

[18] Robin AM. Hydrogen production from coal liquefaction residues. NASA Sti/recon Technical Report N. 1976;77:22687.

[19] Farrokh NT, Askari M, Fabritius T. Investigation of Tabas anthracite coal devolatilization: Kinetics, char structure and major evolved species. Thermochimica Acta. 2017;654:74-80.

[20] Rajabzadeh MA, Ghorbani Z, Keshavarzi B. Chemistry, mineralogy and distribution of selected trace-elements in the Parvadeh coals, Tabas, Iran. Fuel. 2016;174:216-24.

[21] Raygan S, Abdizadeh H, Rizi AE. Evaluation of four coals for blast furnace pulverized coal injection. Journal of Iron and Steel Research, International. 2010;17(3):8-20.

[22] Maurstad O. An Overview of Coal based Integrated Gasification Combined Cycle (IGCC) Technology. MIT, Lab Energy Environ; 2005.

[23] Mrakin A, Selivanov A, Satonin A, Minervina T, Batrakov P, Ermolaev D. Calculation study of

the coal gasification process with steam. In: AIP Conference Proceedings. vol. 2285. AIP Publishing LLC; 2020. p. 020013.

[24] Gungor H, Ozbayoglu, Kasnakoglu, Biyikoglu, Uysal. Determination of Air/Fuel and Steam/Fuel Ratio for Coal Gasification Process to Produce Synthesis Gas; 2011. Available from: https://api.semanticscholar.org/CorpusID:137210361.

[25] Lacson J, J G, Agrawal A. PEP Report 148D-Synthesis Gas Production from Chinese Gasifiers; 2015. Ihs.com.

[26] Baraj E, Ciahotnỳ K, Hlinčík T. Advanced catalysts for the water gas shift reaction. Crystals. 2022;12(4):509.

[27] Ebrahimi P, Kumar A, Khraisheh M. A review of recent advances in water-gas shift catalysis for hydrogen production. Emergent Materials. 2020;3(6):881-917.

[28] Byron SR, Loganathan M, Shantha M. A review of the water gas shift reaction kinetics. Int J Chem React Eng. 2010;8:1-32.

[29] Rozanska X, Valtz A, Riva M, Coquelet C, Wimmer E, Gonzalez-Tovar K, et al. Selective H2S absorption in aqueous tertiary alkanolamine solvents: experimental measurements and quantitative kinetic model. Industrial & Engineering Chemistry Research. 2023;62(29):11480-90.

[30] Kohl AL, Nielsen R. Gas purification. Elsevier; 1997.

[31] Mandal BP, Biswas A, Bandyopadhyay S. Selective absorption of H2S from gas streams containing H2S and CO2 into aqueous solutions of N-methyldiethanolamine and 2-amino-2-methyl-1-propanol. Separation and Purification Technology. 2004;35(3):191-202.

[32] Roshdi S, Bairami A, Abbasi I. Screening and Optimization of Gas Sweetening Process Parameters with MDEA-PZ Solvent using Plackett-Burman Approach. Iranian Journal of Chemical Engineering (IJChE). 2023;20(3):70-89.

[33] Higman C. Gasification. In: Combustion engineering issues for solid fuel systems. Elsevier; 2008. p. 423-68.

[34] Jamekhorshid A, Davani ZK, Salehi A, Khosravi A. Gas sweetening simulation and its optimization by two typical amine solutions: An industrial case study in Persian Gulf region. Natural Gas Industry B. 2021;8(3):309-16.

[35] Kohl AL, Nielsen RB. Gas dehydration and purification by adsorption. Gas Purification. 1997:1022-135.

[36] Kohl A, Nielsen R. Sulfur Recovery Processes In Gas Purification. Houston: Elsevier. 1997:670-730.

[37] Gandhidasan P. Parametric analysis of natural gas dehydration by a triethylene glycol solution. Energy Sources. 2003;25(3):189-201.

[38] Shahabuddin M, Bhattacharya S. Co-gasification characteristics of coal and biomass using co2 reactant under thermodynamic equilibrium modelling. Energies. 2021;14(21):7384.

[39] Cao Y, Gao Z, Jin J, Zhou H, Cohron M, Zhao H, et al. Synthesis gas production with an adjustable H2/CO ratio through the coal gasification process: effects of coal ranks and methane addition. Energy & fuels. 2008;22(3):1720-30.

[40] Ravaghi Ardebili Z, Manenti F, Pirola C, Soares F, Corbetta M, Pierucci S, et al. Influence of the effective parameters on H2: CO ratio of syngas at low-temperature gasification. Chemical Engineering Transactions. 2014;37:253-8.

[41] Bell DA, Towler BF, Fan M. Coal gasification and its applications. William Andrew; 2010.

[42] Rezaiyan J, Cheremisinoff NP. Gasification technologies: a primer for engineers and scientists. CRC press; 2005.

A Supplementary

Table 13. Simulation stream information

	Units	1	2	3	4	5	6	7	8	9	10	11
From					B1	B2	B2	B3	B4		B5	B6
To		B1	B3	B3	B2		B3	B4	B5	B5	B6	B7
Temperature	C	232	24.85	423.52	1050	1050	1050	799.02	1393.3	25.0	230.00	230.00
Pressure	kg/sqcm	24.80	24.80	24.80	24.80	24.8	24.80	24.80	24.80	24.80	24.80	24.80
Mass vapor fraction			1.00	1.00	0.28		0.36	0.74	1.00		1.00	1.00
Mass liquid fraction										1.00		
Mass solid fraction		1.00			0.72	1.00	0.64	0.26				
Mass flows	tonne/hr	21.88	17.51	6.56	21.88	5.09	16.79	40.86	40.86	37.16	78.03	78.03
Mass Fractions (%)												
Coal		100										
Ash					23.26	100						
C					49.08		63.96	26.29				
H_2					12.00		15.64	6.43	5.52		2.89	2.94
N_2					5.60		7.30	3.00	3.00		1.57	1.57
Cl_2												
S					4.43		5.78	2.37				
O_2			100		4.81		6.27	45.42				
CO									53.52		28.03	27.41
CO_2									12.20		6.39	7.37
Methane									0.01			
Water				100	0.80		1.04	16.49	23.22	100	59.79	59.39
H_2S									2.52		1.32	1.32
Volume flow	cum/hr		547.1	839.34	6445		6445	8578.5	14950		7798.7	7800.8

	Unit	12	13	14	15	16	17	18	19	20	21
From		B7	B8	B8	B9	B9	B10	B10	B11	B12	B13
To		B8		B9		B10		B11	B12	B13	
Temperature	C	50.00	50.00	50.00	50.00	50.00	50.00	50.00	200.00	9.31	84
Pressure	kg/sqcm	24.80	24.80	24.80	24.80	24.80	24.80	24.80	24.80	1.40	1.40
Mass vapor fraction		0.41		1.00	1.00	1.00		1.00	1.00	1.00	1.00
Mass liquid fraction		0.59	1.00				1.00				
Mass solid fraction											
Mass flows	tonne/hr	78.03	46.16	31.87	6.76	25.10	0.20	24.91	24.91	24.91	24.91
Mass Fractions (%)											
Coal											
Ash											
C											
H_2		2.9	0.00009	7.19		9.13		9.20	9.20	9.20	9.20
N_2		1.5	0.00001	3.85		4.89		4.92	4.92	4.92	4.92
Cl_2											
S			0.00003								
O_2											
CO		27.41	0.00025	67.11		85.20		85.86	85.86	85.86	85.86
CO_2		7.37	0.00637	18.03	84.94						
Methane				0.01		0.01		0.01	0.01	0.01	0.01
Water		59.39	99.96582	0.61		0.78	100.00				
H_2S		1.32	0.02743	3.20	15.06						
Volume flow	cum/hr	2340		2339.7	157.18	2171.0		2161.2	3172.53	33267.9	131130.0