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Research Article

Syngas Compositions, Cold Gas and Carbon Conversion Efficiencies for Different Coal Gasification Processes and all Coal Ranks

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Abstract

This Paper presents comparison of syngas compositions, for all coal ranks, as produced from different types of coal gasification processes currently in use, namely entrained flow, fluidized bed, and fixed bed gasifiers. Cold gas and carbon conversion efficiencies were investigated. The syngas composition varies with the applied gasification process. The importance of this research arises from the fact that gasifiers produce the environmentally clean fuel required to run any Integrated Gasification Combined Cycle power system. A procedure was conducted to get estimates for bituminous coal. It is important to have knowledge of the chemical reactions which take place in each gasifier and the raw syngas produced from the specific reaction involved to develop an Integrated Coal Gasification Combined Power Generation plant with CO_2 recovery in order to increase the cycle efficiency and mitigate CO_2 emission and other pollutants. The results indicate that the entrained flow gasifier is the dominant one.

Keywords: Syngas; Coal gasification; Cold gas efficiency; Coal conversion efficiency; Gasifiers

Introduction

Gasifiers in an Integrated Gasification Combined Cycle power plant (IGCC) are the heart of the system since they are the producers of the syngas fuel required to operate the plant. Their efficiency and availability are determining factors not only for their design but also for the IGCC system. The study and comparison of different gasifiers are essential for the efficient operation of IGCC plants.

In gasification, organic (carbonaceous) feeds are converted into CO, CO_2, and H_2 by processing the feed at elevated temperatures (>700^0C), without combustion, with a controlled amount of oxygen and/or steam. The produced gas mixture (synthesis gas or syngas) is a fuel. The power generated from the combustion of the syngas, is a source of renewable energy if the obtained gaseous products are produced from a source other than a fossil fuel, e.g. biomass [1].

The main advantage of coal gasification is the utilization of the syngas which is actually more efficient in its burning as compared to the direct combustion of the solid coal because of: (1) the possibility of combustion at higher temperatures, i.e. increasing the thermal efficiency, (2) its use in fuel cells, (3) the possibility to produce methanol and hydrogen, and (4) its conversion via the Fischer–Tropsch (FT) process into a range of synthesis liquid fuels suitable for use in gasoline or diesel engines [1]. In addition, coal is still a virgin resource because of its large reserves in many countries around the world and thus it is greatly more secured than oil and natural gas. It is not subjected to the unexpected price variations in comparison.

The high temperature process produces corrosive ash elements, including metal chlorides and potassium salts, which allow clean gas production from otherwise problematical fuels [1]. However, the ash content in coal is the top important factor in selecting coal since it represents the greatest problem in the operation and performance of a slagging gasifier. Gasifiers need to be efficient for the purpose of increasing the availability of the IGCC system, which is a demanding requirement. It is essential to avoid high ash content in the chosen coal because its melting needs more heat, and hence additional coal and CO are combusted. This increases the amount of CO_2 in the syngas and a reduction in the cold gas efficiency as a consequence of the high ash content.

Coal gasification power plants are cleaner compared to pulverized coal (PC) combustion plants, since they produce less sulphur and nitrogen oxides pollutants. Therefore, gasification is an appealing technology which enables the utilization of both relatively inexpensive and expensive coal reserves, in addition to reducing down the environmental impact. In fact, the increased mounting interest in coal gasification announces two changes in the electricity generation arena: (1) the maturity of coal gasification technology, and (2) the incredibly low air emissions from IGCC power stations, and better lower cost control of greenhouse gases than that for other coal fired plants [1].

The Gasification Process

The real reactions associated with the gasification process are immensely complicated and change with the feed material properties [2].

The gasification of coal comprises three chief steps, as shown in Figure 1: (a) pyrolysis and devolatilization, (b) volatiles cracking and combustion, and (c) char gasification. These processes are explained briefly.

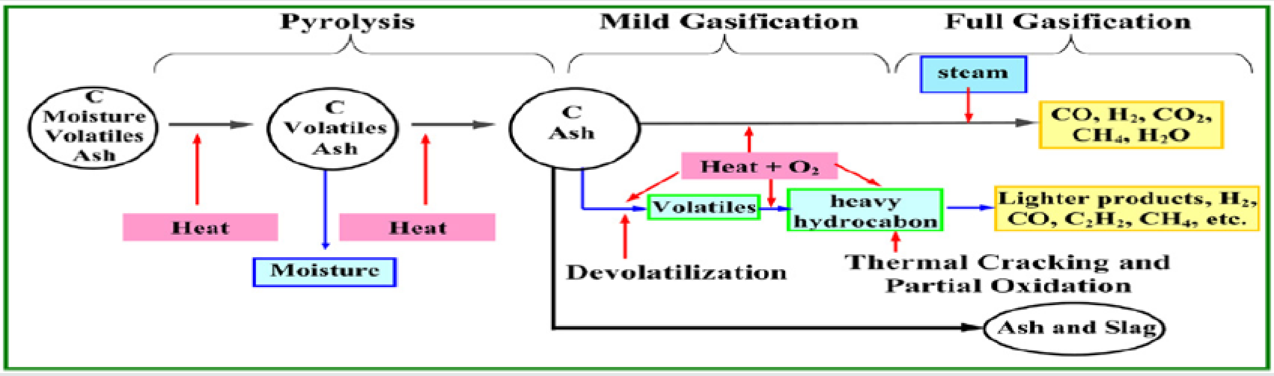

Figure 1: Main steps of coal particles gasification (sulfur and minerals are not included) [2].

Pyrolysis and Devolatilization

The interaction between pyrolysis and gasification under various conditions of heating is depicted in Figure 2. If the heating is slow then the pyrolysis reactions start at about 350°C. The gasification reaction of volatile matters (VM) and char with steam is rather slow at such temperature. The concentration of volatiles outside the coal particle increases quickly, and gasification only takes place after devolatilization is accomplished. However, in case the heating rate is high, then both pyrolysis and gasification occur concurrently, so that high concentration of volatiles is never permitted to build up. This explains why a clean gas in such a short time is produced from high-temperature entrained-flow gasifiers. In Ref. [3], it is indicated that in contrast with a counter flow moving-bed process, where lump coal is employed, the rate of heating is slow and a high volatiles concentration grows up and discarded unreacted from the reactor by the syngas.

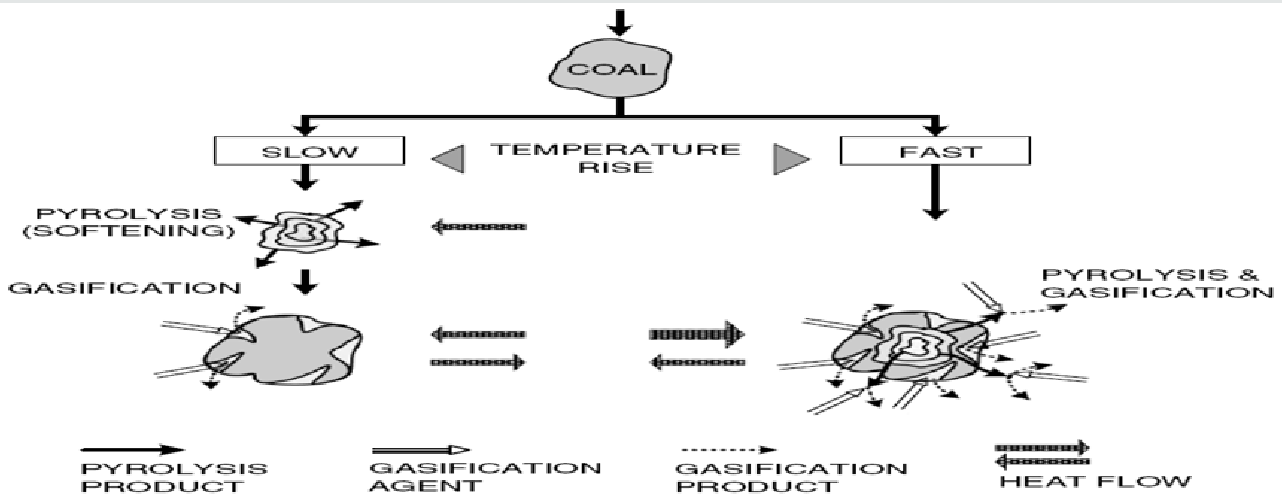

Figure 2: Effect of heating rate on the gasification process [3].

Volatiles Combustion

The devolatilization of coal produces multi species, which include tars, hydrocarbon liquids, and gases such as CH_4, CO, CO_2, H_2, H_2O, HCN, and so on. These react with the oxidant surrounding the coal particle. The extent to which the oxidant is completely or partially depleted depends on the quantities of volatiles produced [3].

In combustion, where there is excess of oxygen, the volatiles are completely combusted. The moderating effect of carbon dioxide and water vapour reduces the temperature. In gasification the recycled gas contains notable amounts of carbon monoxide and hydrogen (up to 90% for an oxygen-blown gasifier) which causes tremendously high local temperatures, in case it comes into contact with the oxidant [3].

Coal Gasification

Gasification commences under shortage of oxygen. Coal is first heated in a closed chamber where it undertakes a pyrolysis process at temperatures over 400°C. During pyrolysis, hydrogen rich VM is released, together with tar, phenols, and gaseous hydrocarbons. Then, char is gasified, with the liberation of gases, tar vapours, and solid residues. The ruling reactions subsist of partial oxidation of char, which produces a syngas with high fractions of H_2 and CO. The process happens at temperatures between 800 and 1800°C. Exact operating conditions depend on coal type, properties of the resulting ash, and the gasification technology. The oxidant is the highly important variable in the gasification process. It can be either air or pure oxygen in case the process includes an air separation unit (ASU) for O_2 production. The deployment of an ASU adds cost to the power plant.

If the coal is heated externally, the process is termed "allothermal," while "autothermal" process assumes heating of coal by means of exothermal chemical reactions undergoing inside the gasifier. Oxygen and water molecules oxidize the coal and produce a gaseous mixture of CO_2, CO, H_2O vapour, H_2, and CH_4. Some by-products like tar and phenols are also possible end products, depending on the type of the employed gasification technology. The likely wanted end product is usually syngas (i.e., a combination of H_2 + CO), but the released coal gas may be further refined to produce extra quantities of H_2, according to: $3C\ (coal) + O_2 + H_2O \rightarrow H_2 + 3CO$ [4].

Char Gasification

As only char and ash left, the char particles sustain two important endothermic, heterogeneous gasification reactions: (1) the Boudouard reaction: $C(s) + CO_2 \leftrightarrow 2CO$ (or, more specifically, the reverse Boudouard reaction, and it is also known as carbon dioxide-char gasification), and (2) the $C(s) + H_2O\ (g) \rightarrow CO + H_2$ or $C(s) + 2H_2O\ (g) \rightarrow CO_2 + 2H_2$ reactions (also named steam-char gasification), where s and g refer to solid and gas, respectively. Both reactions are endothermic [2].

The steam-char reaction is the supreme contributor to the production of both H_2 and CO, which are the primary reactive constituents of the syngas [2].

Water-Gas Shift (WGS)Process Inside Gasifiers

The water-gas shift reaction is an equilibrium process: $CO + H_2O\ (g) \leftrightarrow CO_2 + H_2$. The forward reaction is exothermic, in which CO and steam are converted to H_2 and CO_2. The forward reaction is energetic at temperatures less than 700°C. At higher temperatures, near 1000°C, the net reaction is slow and negligible. More than 1200°C, the backward reaction becomes commanding. The reaction rate of the WGS is usually slow without using catalysts; however, in the gasifier, the reaction rate is usually enhanced by the catalytic effect of metallic components in coal. In gasifiers which utilize the quench method to cool down the syngas to near 200°C, the residence time is very short to achieve any remarkable forward WGS reaction, despite that the equilibrium constant value is large at low temperatures, because the catalytic effect from metals in coal is feeble in the quenched syngas since most of the metals have become molten slag, which is extracted during the gasification process, before quenching takes place [2].

Methanation

The methanation reaction [$C + 2H_2 \rightarrow CH_4$] is predominantly exothermic and pressure favourable, so it is generally inactive in high-temperature atmospheres, for instance in high-temperature entrained flow gasifiers [2].

Types of Gasifiers

Detailed descriptions of gasifier types and their operation can be found in many references. Operating data and innovative gasifiers studied prior to the 1980s are reported in some early studies. Recent approaches to gasification such as catalytic, molten salt, plasma, or secondary heated systems are dealt with elsewhere. Only the major gasifiers in use today are described. It is suggested that the foremost gasifier types are moving bed, fluidized bed, and entrained flow ones [5].

Fixed Bed Gasifier

A fixed bed gasifier is illustrated in Figure 3 The coal to ash and gas production schemes along the gasifier as the temperature varies is shown. These gasifiers are counter current flow ones; coal is fed at the top and the oxidant from the bottom. As the coal slowly proceeds down through the gasifier, it is gasified and the resulting ash drops out of the bottom. The counter current flow design allows the utilization of the heat of reaction from the gasification reactions to preheat the coal before its entrance to the gasification reaction zone. Consequently, the temperature of the syngas exiting the gasifier is remarkably less than the temperature required for total conversion of coal [6].

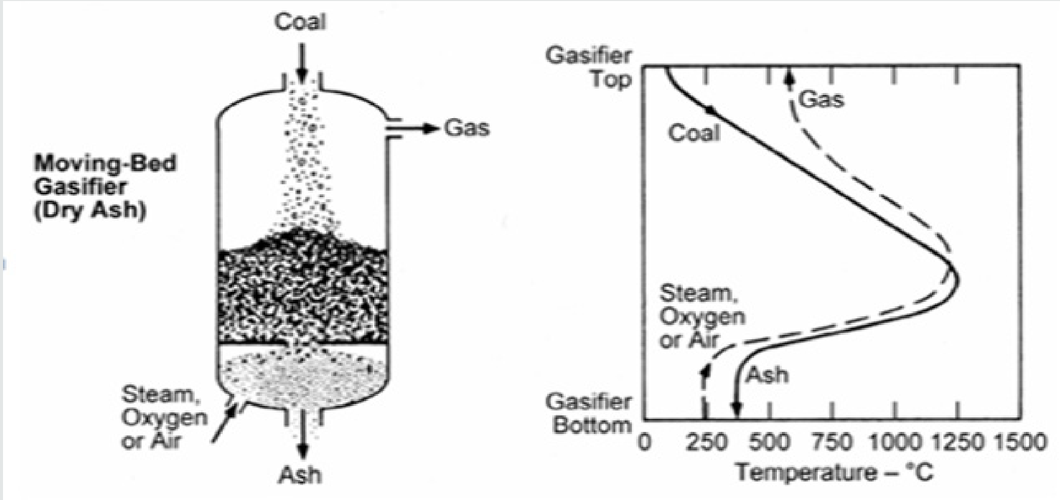

Figure 3: A fixed bed gasifier [6].

These features are notable in such gasifiers: the residence time of coal inside may be of the order of hours, low oxidant requirements, relatively high content of CH_4 in the resulting gas, production of hydrocarbon liquids, such as oils and tars, high cold gas thermal efficiency when including the heating value of the hydrocarbon liquid, limited ability to handle fines, and special requirements for handling caking coal. Fixed bed gasifiers are still in use and have long industrial experience as the so named Lurgi type. However, reliable but are not suitable for one large scale gasifier. Recently a Lurgi of 1600 ton/day capacity was manufactured [7].

Fluidized Bed Gasifier

Figure 4 shows a fluidized bed gasifier. The figure illustrates how coal is converted into ash and the gas production across the gasifier as the temperature goes up. It is a back-mixed or well-stirred reactor where there is a consistent mixture of fresh coal particles mixed with older ones, some of which are partially gasified, and some are totally gasified. The mixing regime allows consisting temperatures throughout the bed. The gas flow into the reactor (oxidant, steam, recycled syngas) must be adjusted such that to suspend coal particles within the bed but not too high to entrain them out. As the gasified coal particles gets smaller and lighter, they will escape from the gasifier. In order to avoid particle agglomeration, it is important to ensure that the temperatures within the bed to be lower than the initial ash fusion temperature of coal [6].

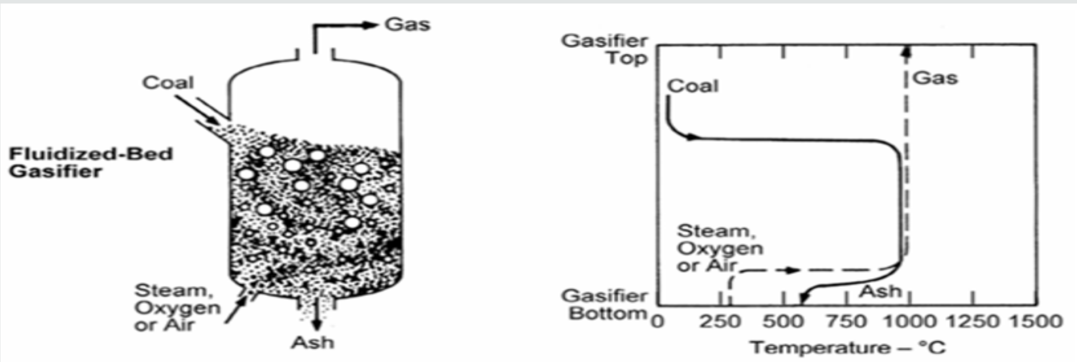

Figure 4: A fluidized bed gasifier [6].

A cyclone downstream the gasifier will capture the larger particles that are entrained out and return them back to the bed. The residence time of coal particles in these gasifiers is shorter than that in a moving bed one [6]. The main characteristics of these gasifiers are extensive solids recycling, uniform and moderate temperature, and moderate oxygen and steam requirements. Fluidized-bed gasifiers have been developed for the gasification of low-grade fuels or feed stock. The working principle of the fluidized bed embraces even distribution of oxidant through the reactor. Gas bubbles tend to flow via the less congested area, and this results in the existence of a dead zone inside the reactor. This creates difficulties in scaling up design and operation. Most distinguished fluidized-bed examples are fluidized bed boiler and waste pyrolysis plants [7].

Entrained Flow Gasifier

Figure 5 shows a diagram of an entrained flow gasifier. The figure gives the coal gas conversion and gas production along the reactor as a function of temperature. Co-current flow of pulverized coal and oxidant are injected into the reactor. The coal is rapidly heated up and reacts with the oxidant. The residence time in these gasifiers is of the order of seconds. Because of this short time, such gasifiers must perform at high temperatures in order to attain high carbon conversion efficiency. Therefore, shows that the majority of entrained flow gasifiers employ oxygen rather than air and operate above the slagging temperature of coal [6].

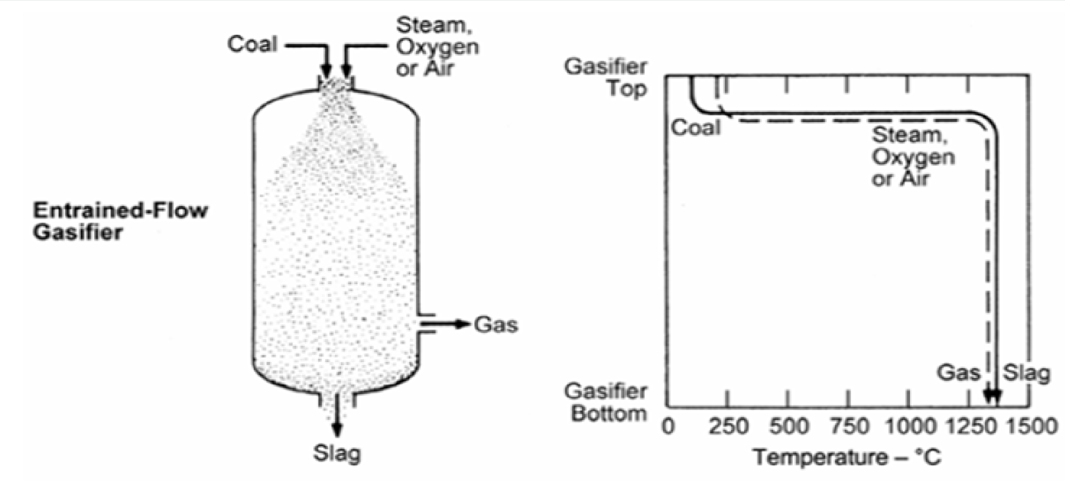

Figure 5: A fluidized bed gasifier [6].

Properties of entrained flow gasifiers include: high-temperature slagging performance, entrainment of some molten slag in the raw syngas, relatively large oxidant requirements, vast chunk of sensible heat in the raw syngas, and the potential to gasify all coal ranks, caking characteristics, or degree of fines.

The processes that need a high throughput capacity in a single reactor generally use entrained bed type, as in IGCC, since the reactor size can be reduced by the fast residence time (typically less than 5 sec) as well as by high pressure. Although large scale operation of entrained bed gasifiers have been successfully operated commercially, however, the experience is not long enough as in the case of fixed or fluidized bed gasifiers. It is concluded that the foremost disadvantage of entrained bed gasifier is its high capital cost due to the compact configuration of parts [7].

Concluding Remarks on Gasifiers

From the above discussions it is concluded that the favourable is the entrained flow one because:

a) The residence time is too short and in the order of second so it must operate at elevated temperatures to attain high carbon conversion efficiency.

b) It produces a clean gas in a short time as a result of operating at high temperature.

c) Large scale performance due to the short residence time and high carbon conversion efficiency, thus increasing both the throughput coal and yield abundantly.

d) It increases the gas velocity which can reach 80–100 m/s.

e) The manufacturing cost is less compared to other types of gasifiers.

f) Low hydrocarbon because of the high temperature.

g) High CO_2 capture because of the high CO in syngas.

h) None or very little tar formation because it is a downdraft gasifier.

i) The radiant syngas cooling can increase the cycle efficiency by 4 – 5% over full quench types.

Gasifiers need further improvements and developments in order to increase their efficiencies and performance for more availability of IGCC systems.

Methodology of Calculations

During the gasification of solid carbon, whether in the form of coal, coke, or char, the main chemical reactions are those associated with C, CO, CO_2, H_2, H_2O (or steam), and CH_4. These reactions are:

Combustion reactions

$C + ½O_2 = CO$ - 111 MJ/kmol (1)

$CO + ½O_2 = CO_2$ - 283 MJ/kmol (2)

$H_2 + ½O_2 = H_2O$ - 242 MJ/kmol (3)

The Boudouard reaction

$C + CO_2 = 2CO + 172$ MJ/kmol (4)

The water gas reaction

$C + H_2O = CO + H_2 + 131$ MJ/kmol (5)

The methanation reaction

$C + 2H_2 = CH_4 + 75$ MJ/kmol (6)

As reactions with free oxygen are all complete under gasification conditions, reactions (1), (2) and (3) do not need to be considered in determining an equilibrium syngas composition. The three heterogeneous (i.e. gas and solid phase) reactions (4), (5) and (6) are sufficient. In general, we are concerned with situations where the carbon conversion is also essentially complete. Under these circumstances, Equations (4), (5), and (6) can be reduced to these two homogeneous gas reactions:

The water gas shift reaction

$CO + H_2O = CO_2 + H_2 + 41$ MJ/kmol (7)

The steam methane reforming reaction

$CH_4 + H_2O = CO + 3H + 206$ MJ/kmol (8)

Note that by subtracting the moles and heat effects from reaction (4) from those in reaction (5), one obtains reaction (7), and by subtracting reaction (6) from (5), one obtains reaction (8). Thus reactions (7) and (8) are implicit in reactions (4), (5), and (6) – but not the other way around. Three independent equations always contain more information than two. Reactions (1), (4), (5), and (6) describe the four ways in which a carbonaceous or hydrocarbon fuel can be gasified. Reaction (4) is important for the production of pure CO when gasifying pure carbon with an O_2/CO_2 mixture. Reaction (5) plays a predominant role in the water gas process. Reaction (6) is the basis of all hydrogenating gasification processes. But most gasification processes rely on a balance between reactions (1) (partial oxidation) and (5) (water gas reaction). For real fuels (including coal, which also contains hydrogen), the overall reaction can be written as:

$C_nH_n + n/2\ O_2 = nCO + m/2\ H_2$ (9)

Where

- For gas, as pure methane, m = 4 and n = 1, hence m/n = 4
- For oil, m/n = 2, hence m = 2 and n = 1
- For coal, m/n = 1, hence m = 1 and n = 1.

Gasification temperatures are so high that, thermodynamically as well as in practice, no hydrocarbons other than methane can be present in any appreciable quantity.

Thermodynamic equilibrium: As an example: Equations (1) and (5) produce H_2 and CO which absorbs and releases heat

$C + ½O_2 = CO - 111$ MJ/kmol (10)

$C + H_2O = CO + H_2 + 131$ MJ/kmol (11)

The molar weight and mass flow rate ton/day (TPD) of each component in both sides of Eqs. (10) and (11) can be determined and written under each equation for clarity.

Equation (10) releases heat, and Eq. (11) absorbs heat. The heat released is used to heat a fire tube boiler or utilized in another gasification application.

The above methodology is used in what follows to conduct detailed calculations of the syngas composition, cold gas efficiency, and carbon conversion efficiency, but for one coal type, bituminous coal, which is the mostly used in power plants. The purpose of this is to show the step by step of such calculation procedures. This is done for the three studied gasification processes. The results for other coals are given briefly following the same procedures as in the case of bituminous coal.

Data and Assumptions

To perform the calculations, numerical data and assumptions should be made. The coal ranks considered cover the high grade ones (anthracite and bituminous) and low ranks (sub-bituminous and lignite). Mass percentages of constituents of coals are depicted in Table 1 [5].

Table 1: Coal compositions at combustion.

Composition / % Coal type	C	H	O	N	S	Moisture	Ash
Anthracite	76.1	1.8	1.8	0.6	0.6	5.4	13.7
Bituminous	80.7	4.5	2.4	1.1	1.8	3.3	6.2
Sub bituminous	58.8	3.8	12.2	1.3	0.3	19.6	4
Lignite	42.4	2.8	12.4	0.7	0.7	34.8	6.2

To get coal chemical compositions, we must calculate mole fractions of all species and hence their normalized values with respect to carbon, and these are presented in Table 2. Coal compositions as extracted from the normalized mole fractions, in Table 2, are shown in Table 3.

Equations for complete combustion of coals are indicated in Table 4.

Table 2: Mole fractions and normalized values with respect to carbon of coal constituents.

Coal	Mole fraction and normalized values in ( )				
	C	H	O	N	S
Anthracite	6.3416	1.8	0.1125	0.0428	0.0187
	(1)	(0.2838)	(0.0067)	(0.0067)	(0.0029)
Bituminous	6.725	4.5	0.15	0.0785	0,0562
	(1)	(0.6691)	(0.0223)	(0.0116)	(0.0083)
Sub- bituminous	4.9	3.8	0.7625	0.0928	0.0093
	(1)	(0.7755)	(0.1566)	(0.0189)	(0.0019)
Lignite	3.533	2.8	0.775	0.05	0.0218
	(1)	(0.7825)	(0.2193)	(0.0141)	(0.0061)

Note: Molar fractions are estimated by dividing the mass percentage of each species (from Table 1) by its atomic weight. Example: for bituminous coal, the mole fraction of C= 76.1/12= 6.6735, H= 4.5/1= 4.5, S= 1.8/32= 0.0083. Normalized values are obtained by dividing the mole fraction of the species by that of carbon. For example: for bituminous coal, C= 7.625/7.625= 1, and N= 0.0785/7.625= 0.0116.

Table 3: Chemical compositions of coal ranks. Note: coal compositions are extracted from the normalized values given in Table 2.

Coal	Composition
Anthracite	$C\,H_{0.28}\,O_{0.0177}7\,N_{0.0067}\,S_{0.0029}$
Bituminous	$C\,H_{0.67}\,O_{0.022}\,N_{0.0116}\,S_{0.008}$
Sub- bituminous	$C\,H_{0.775}\,O_{0.155}\,N_{0.0189}\,S_{0.0019}$
Lignite	$C\,H_{0.8}\,O_{0.22}\,N_{0.014}\,S_{0.006}$

Table 4: Equations for complete combustion of coals.

Coal	Complete combustion equation
Anthracite	$C\,H_{0.28}\,O_{0.0177}\,N_{0.0067}\,S_{0.0029} + 1.064\,(O_2 + 3.78N_2) = CO_2 + 0.14\,H_2O + 0.0029\,SO_2 + 4.025\,N_2$
Bituminous	$CH_{0.67}\,O_{0.022}\,N_{0.0116}\,S_{0.008} + 1.1645\,(O_2 + 3.78N_2) = CO_2 + 0.335\,H_2O + 0.008\,SO_2 + 4.4\,N_2$
Sub- bituminous	$CH_{0.775}\,O_{0.155}\,N_{0.0189}\,S_{0.0019} + 1.118\,(O_2 + 3.78N_2) = CO_2 + 0.3875\,H_2O + 0.0019\,SO_2 + 4.235\,N_2$
Lignite	$CH_{0.8}\,O_{0.22}\,N_{0.014}\,S_{0.006} + 1.096\,(O_2 + 3.78N_2) = CO_2 + 0.4\,H_2 + 0.006\,SO_2 + 4.15\,N_2$

The heating values used in calculations of cold gas efficiencies are listed in Table 5.

Table 5: Heating values of coals and gases.

Species	Heating values (kJ/kg)
Anthracite coal	33300 (HHV)
Bituminous coal	27800 (HHV)
Sub- bituminous coal	23600 (HHV)
Lignite coal	16800 (HHV)
H_2	121000 (LHV)
CO	10095 (LHV)
CH_4	49995 (LHV)

Note: HHV= High Heating Value, and LHV= Low Heating Value.

For all present calculations, we assumed a flow rate of coal in gasifiers= 2500 TPD. Oxygen is blown in gasifiers and the pressure= 30 atm.

The chemical equation in gasifiers is

$$CH_{0.67}\,O_{0.022}\,N_{0.0116}\,S_{0.008}. + a\,H_2O + b\,O_2 = e\,CO + f\,H_2 + g\,COS + j\,H_2S + k\,CO_2 + l\,CH_4 + m\,H_2O$$

Where: a, b, c.....etc are fractions determined for each coal and each gasifier.

Detailed Calculations for Bituminous Coal

In the following calculations the molar weight of carbon in coal M_c= 100/6.725= 14.869 gm/mole. From the mass weights in Table 1, moisture and ash flow rates are 82.5 (= 0.033x2500) and 155 TPD (= 0.062x2500), respectively.

Entrained Flow Gasification

Reactions in gasifier:

A. Pyrolysis and devolatilization of coal

C_s = 0.3345 H_2 + 0272 H_2O+ 0.0058 N_2 + 0.008H_2S + 0.0115 O_2 (12)

14.869 0.669 0.4896 0.1624 0.272 0.3568

2500 TPD 112.5 82.5 27.5 47.812 60

H_2 + S = H_2S (13)

2 32 34

2.812 TPD 45 47.812

B. Gasification

3C_s + H_2O + O_2 = 3CO + H_2 (14)

44.607 18 32 84 2

2500 TPD 1008.81 1793.44 4707.781 112.09

C. Combustion

CO + 0.5 O_2 = CO_2 (15)

28 16 44

536.48 TPD 306.56 843.04

D. Water from partial combustion

H_2 + 0.5 O_2 = H_2O (Water with slag) (16)

2 16 18

7.5 TPD 60 67.5

From above calculations, $\dot{m}_{O2}$= 2100 TPD (= 84% by weight of coal), and $\dot{m}_{CO}$= 1008.81 TPD (=40.352% of slurry feed)

a) Mass flow rates of gasses in syngas ($\dot{m}_{gas}$) TPD

$\dot{m}_{CO2}$= 843.04 $\dot{m}_{CO}$= 4171.301 $\dot{m}_{H2}$= 214.278 $\dot{m}_{N2}$= 27.5 $\dot{m}_{H2S}$= 47.812

These mass flow rates are used to determine the CGη.

$CH_{0.67}O_{0.022}N_{0.0116}S_{0.008}$. + 0.333 H_2O + 0.39 O_2 = 0.886 CO + 0.637 H_2 + 0.008 H_2S + 0.114 CO_2 + 0.006 N_2+ 0.022 H_2O (17)

Total moles of syngas = Σ fractions in the RHS of Eq. (17) = 1.673

Y_{gas} (%) = (number of moles in species / total moles in syngas) x 100

Y_{CO2}= 6.814 Y_{CO}= 52.958 Y_{H2}= 38.075 Y_{N2}= 0.358 Y_{H2S}= 0.478

b) Cold gas efficiency (CGη)

CGη is estimated by considering only H_2, CO, and CH_4 in syngas.

ΔH_C = 300088.4 {= (214.278x1000 / 24x60x60) x 121000} + 487375.97 = 787464.37 kW

CGη = [ΔHc / ($\dot{m}_c$ (= 2500 TPD) × HHV) $_{Coal}$] ×100 = [787464.3 / 963541.67 (= {(2500x1000/24x60x60) x 333000}] ×100= 81.726 %

c) Carbon conversion efficiency (CCη)

CCη = ṁ carbon in coal / ṁ carbon in syngas = [(2500 / 2500) × 100 = 100 %

Fluidized Bed Gasification

Reactions in gasifier:

A. Pyrolysis and devolatilization: Equation (12) still applies.

B. Gasification and combustion

3C_s + H_2O + O_2 = 3CO + H_2 (18)

44.607 18 32 84 2

2265.2 TPD 914.062 1625 4265.625 101.562

C. Water from partial combustion: Equation (16) is the same.

D. Water gas shift

CO + H_2O = CO_2 + H_2 (19)

28 18 44 2

911.459 TPD 585.938 1432.293 65.104

E. Methanation

C_S + 2H_2 = CH_4 (20)

14.869 4 16

159.8 TPD 42.988 171.955

The above results reveal that $\dot{m}_{O2}$ and $\dot{m}_{steam}$ (steam feed) are 1750 and 1500 TPD, i.e. 70 and 60% by weight of coal, respectively.

a) $\dot{m}_{gas}$ (TPD)

$\dot{m}_{CO2}$= 1432.293 $\dot{m}_{CO}$= 3354.166 $\dot{m}_{H2}$= 228.678 $\dot{m}_{N2}$= 27.5 $\dot{m}_{CH4}$= 171.955 $\dot{m}_{Steam}$= 82.5

$CH_{0.67}O_{0.022}N_{0.0116}S_{0.008.}$ + 0.495 H_2O + 0.302 O_2 = 0.712 CO + 0.68 H_2 + 0.064 CH_4 + 0.193 CO_2 + 0.027 H_2O + 0.006 N_2 (21)

Y_{gas} (%):

Total moles of syngas = 1.682

Y_{CO2}= 11.474 Y_{CO}= 42.33 Y_{H2}= 40.428 Y_{CH4}= 3.805 Y_{N2}= 0.356 Y_{H2S}= 0 Y_{Steam}= 1.605

b) CGη

ΔH_C = 320255.07 + 391901.69 + 99501.044 = 811657.8 kW

- CGη = [ΔH_C / (ṁ × HHV) $_{Coal}$] × 100 = [811657.8 / 963541.67] ×100= 84.237 %

c) CCη

CCη = = [2425 / 2500] × 100 = 97%

Fixed Bed Gasification

Reactions in gasifier:

A. Pyrolysis and devolatilization: Equations (12) and (13) are applicable.

B. Gasification and combustion

$3C_S + H_2O + O_2 = 3CO + H_2$ (22)

44.607 18 32 84 2

1847.008 TPD 745.312 1325 3478.125 82.812

C. Water from partial combustion: Equation (16) applies

D. Steam Gasification

$C_S + 2H_2O = CO_2 + 2H_2$ (23)

14.869 36 44 4

105.193 TPD 254.688 311.285 28.298

E. Direct methanation

$C_S + 2H_2 = CH_4$ (24)

14.869 4 16

497.799 TPD 133.916 535.663

Here $\dot{m}_{O2}$ and $\dot{m}_{steam}$ (steam feed) are 1325 and 1000 TPD, i.e. 53 and 40% by weight of coal, respectively.

a) $\dot{m}_{gas}$ (TPD)

$\dot{m}_{CO2}$= 311.285 $\dot{m}_{CO}$= 3478.125 $\dot{m}_{H2}$= 79.38 $\dot{m}_{N2}$= 27.5 $\dot{m}_{CH4}$= 535.663 $\dot{m}_{H2}$ = 47.812 $\dot{m}_{Steam}$= 82.5

$CH_{0.67} O_{0.022} N_{0.0116} S_{0.008.} + 0.33 H_2O + 0.246 O_2 = 0.739 CO + 0.236 H_2 + 0.199 CH_4 + 0.008 H_2S + 0.042 CO_2 + 0.006 N_2 + 0.027 H_2O$ (25)

Y_{gas} (%):

Total moles of syngas = 1.257

Y_{CO2}= 3.341 Y_{CO}= 58.79 Y_{H2}= 18.775 Y_{CH4}= 15.831 Y_{N2}= 0.477 Y_{H2S}= 0.636 Y_{H2O}= 2.148

b) CGη

ΔH_C = 111171.55 + 406384.51 + 309959.16 = 827515.22 kW

CGη = [ΔH_C/ ($\dot{m}$ × HHV) $_{Coal}$] × 100 = [827515.22 / 963541.67] × 100= 85.882 %

c) CCη

CCη = = [2450 / 2500] × 100 = 98 %

Calculations for Other Coals

Entrained Flow Gasification

Anthracite coal

Mass flow rate of oxygen blown in gasifier ($\dot{m}_{O2}$) = 1980.297 TPD

Mass flow rate of water slurry ($\dot{m}_{water}$) = 951.25 TPD

$\dot{m}_{gas}$ (TPD):

$\dot{m}_{CO2}$= 795.262 $\dot{m}_{CO}$= 3933.091 $\dot{m}_{H2}$= 144.132 $\dot{m}_{N2}$= 15 $\dot{m}_{H2S}$= 15.938 $\dot{m}_{Steam}$ = 135

Chemical equation:

$CH_{0.28} O_{0.0177} N_{0.0067} S_{0.0029} + 0.333 H_2O + 0.39 O_2 = 0.886 CO + 0.454 H_2 + 0.003 H_2S + 0.114 CO_2 + 0.003 N_2 + 0.047 H_2O$ (26)

a) Y_{gas} (%):

All moles of syngas = 1.507

Y_{CO2}= 7.564 Y_{CO}= 58.792 Y_{H2}= 30.126 Y_{N2}= 0.2 Y_{H2S}= 0.2 Y_{H2O}= 3.118

Sub bituminous coal:

$\dot{m}_{O2}$ = 1530.112 TPD

$\dot{m}_{water}$ = 735 TPD

$\dot{m}_{gas}$ (TPD):

$\dot{m}_{CO2}$= 614.473 $\dot{m}_{CO}$= 3038.971 $\dot{m}_{H2}$= 138.073 $\dot{m}_{N2}$= 32.5 $\dot{m}_{H2S}$= 7.969 $\dot{m}_{Steam}$ = 490

a) Chemical equation:

$C H_{0.775} O_{0.155} N_{0.0189} S_{0.0019} + 0.333 H_2O + 0.39 O_2 = 0.886 CO + 0.563 H_2 + 0.002 H_2S + 0.114 CO_2 + 0.01 N_2 + 0.222 H_2O$ (27)

Total moles of syngas = 1.797

Y_{CO2}= 6.344 Y_{CO}= 49.304 Y_{H2}= 31.33 Y_{N2}= 0.556 Y_{H2S}= 0.111 Y_{H2O}= 12.354

Lignite coal:

$\dot{m}_{O2}$ = 1103.346 TPD

$\dot{m}_{water}$ = 530 TPD

$\dot{m}_{gas\ (TPD)}$:

$\dot{m}_{CO2}$= 443.09 $\dot{m}_{CO}$= 2191.367 $\dot{m}_{H2}$= 89.045 $\dot{m}_{N2}$= 17.5 $\dot{m}_{H2S}$= 18.594 $\dot{m}_{Steam}$ = 870

a) Chemical equation:

$C H_{0.8} O_{0.22} N_{0.014} S_{0.006} + 0.333 H_2O + 0.39 O_2 = 0.886 CO + 0.504 H_2 + 0.006 H_2S + 0.114 CO_2 + 0.007 N_2 + 0.547 H_2O$ (28)

b) Y_{gas} (%):

Total moles of syngas = 2.064

Y_{CO2}= 5.523 Y_{CO}= 42.926 Y_{H2}= 24.418 Y_{N2}= 0.339 Y_{H2S}= 0.29 Y_{H2O}= 26.502

Fluidized Bed Gasification

Anthracite coal:

($\dot{m}_{O2}$) = 1650.248 TPD

($\dot{m}_{water}$) = 1414.498 TPD

$\dot{m}_{gas}$ (TPD):

$\dot{m}_{CO2}$= 1350.649 $\dot{m}_{CO}$= 3162.975 $\dot{m}_{H2}$= 156.040 $\dot{m}_{N2}$= 15 $\dot{m}_{CH4}$= 162.007 $\dot{m}_{Steam}$ = 135

a) Chemical equation:

C $H_{0.28}$ $O_{0.0177}$ $N_{0.0067}$ $S_{0.0029}$ + 0.495 H_2O + 0.325 O_2 = 0.712 CO + 0.492 H_2 + 0.064 CH_4 + 0.193 CO_2 + 0.003 N_2 + 0.047 H_2O (29)

b) Y_{gas} (%):

Total moles of syngas = 1.511

Y_{CO2}= 12.773 Y_{CO}= 47.121 Y_{H2}= 32.561 Y_{N2}= 0.198 Y_{CH4}= 4.235 Y_{H2O}= 3.11

Sub bituminous coal:

$\dot{m}_{O2}$ = 1275.093 TPD

Mass flow rate of steam for gasification ($\dot{m}_{steam}$) = 1092 TPD

$\dot{m}_{gas}$ (TPD):

$\dot{m}_{CO2}$= 1043.603 $\dot{m}_{CO}$= 2443.928 $\dot{m}_{H2}$= 147.018 $\dot{m}_{N2}$= 32.5 $\dot{m}_{CH4}$= 125.178 $\dot{m}_{Steam}$ = 490

a) Chemical equation:

$CH_{0.775}$ $O_{0.155}$ $N_{0.0189}$ $S_{0.0019}$ + 0.495 H_2O + 0.325 O_2 = 0.712 CO + 0.6 H_2 + 0.064 CH_4 + 0.193 CO_2 + 0.01 N_2 + 0.222 H_2O (30)

b) Y_{gas} (%):

Total moles of syngas = 1.801

Y_{CO2}= 10.716 Y_{CO}= 39.533 Y_{H2}= 33.314 Y_{N2}= 0.555 Y_{CH4}= 3.553 Y_{H2O}= 12.326

Lignite coal:

$\dot{m}_{O2}$ = 919.455 TPD

$\dot{m}_{water}$ = 788.104 TPD

$\dot{m}_{gas}$ (TPD):

$\dot{m}_{CO2}$= 752.53 $\dot{m}_{CO}$= 1762.288 $\dot{m}_{H2}$= 96.251 $\dot{m}_{N2}$= 17.5 $\dot{m}_{CH4}$= 90.264 $\dot{m}_{Steam}$ = 870

a) Chemical equation:

$CH_{0.8}$ $O_{0.22}$ $N_{0.014}$ $S_{0.006}$ + 0.495 H_2O + 0.325 O_2 = 0.712 CO + 0.544 H_2 + 0.064 CH_4 + 0.193 CO_2 + 0.007 N_2 + 0.547 H_2O (31)

b) Y_{gas} (%):

Total of moles of syngas = 2.067

Y_{CO2}= 9.337 Y_{CO}= 34.446 Y_{H2}= 26.318 Y_{N2}= 0.338 Y_{CH4}= 3.096 Y_{H2O}= 26.463

Fixed Bed Gasification

Anthracite coal:

$\dot{m}_{O2}$ = 1249.473 TPD

$\dot{m}_{steam}$ = 942.999 TPD

$\dot{m}_{gas}$ (TPD):

$\dot{m}_{CO2}$= 293.541 $\dot{m}_{CO}$= 3279.868 $\dot{m}_{H2}$= 16.97 $\dot{m}_{N2}$= 15 $\dot{m}_{CH4}$= 504.981 $\dot{m}_{Steam}$ = 135 $\dot{m}_{H2S}$= 15.938

a) Chemical equation:

$CH_{0.28}$ $O_{0.0177}$ $N_{0.0067}$ $S_{0.0029}$ + 0.33 H_2O + 0.246 O_2 = 0.739 CO + 0.053 H_2 + 0.199 CH_4 + 0.042 CO_2 + 0.003 N_2 + 0.047 H_2O + 0.003 H_2S (32)

b) Y_{gas} (%):

Total moles of syngas = 1.086

Y_{CO2}= 3.867 Y_{CO}= 68.047 Y_{H2}= 4.88 Y_{N2}= 0.276 Y_{CH4}= 18.324 Y_{H2O}= 4.327 Y_{H2S}= 0.276

Sub bituminous coal:

$\dot{m}_{O2}$ = 965.427 TPD

$\dot{m}_{steam}$ = 728.624 TPD

$\dot{m}_{gas}$ (TPD):

$\dot{m}_{CO2}$= 226.81 $\dot{m}_{CO}$= 2534.247 $\dot{m}_{H2}$= 39.819 $\dot{m}_{N2}$= 32.5 $\dot{m}_{CH4}$= 390.183 $\dot{m}_{Steam}$ = 490 $\dot{m}_{H2S}$= 7.969

a) Chemical equation:

$CH_{0.775}$ $O_{0.155}$ $N_{0.0189}$ $S_{0.0019}$ + 0.33 H_2O + 0.246 O_2 = 0.739 CO + 0.162 H_2 + 0.199 CH_4 + 0.042 CO_2 + 0.01 N_2 + 0.222 H_2O + 0.002 H_2S (33)

b) Y_{gas} (%):

Total moles of syngas = 1.376

Y_{CO2}= 3.052 Y_{CO}= 53.706 Y_{H2}= 11.773 Y_{N2}= 0.726 Y_{CH4}= 14.462 Y_{H2O}= 16.133 Y_{H2S}= 0.145

Lignite coal:

$\dot{m}_{O2}$ = 696.159 TPD

$\dot{m}_{steam}$ = 525.403 TPD

$\dot{m}_{gas}$ (TPD):

$\dot{m}_{CO2}$= 163.55 $\dot{m}_{CO}$= 1827.416 $\dot{m}_{H2}$= 18.195 $\dot{m}_{N2}$= 17.5 $\dot{m}_{CH4}$= 281.356 $\dot{m}_{Steam}$ = 870 $\dot{m}_{H2S}$= 18.594

a) Chemical equation:

$CH_{0.8}$ $O_{0.22}$ $N_{0.014}$ $S_{0.006}$ + 0.33 H_2O + 0.246 O_2 = 0.739 CO + 0.103 H_2 + 0.199 CH_4 + 0.042 CO_2 + 0.007 N_2 + 0.547 H_2O + 0.006 H_2S (34)

b) Y_{gas} (%):

Total moles of syngas = 1.643

Y_{CO2}= 2.556 Y_{CO}= 44.978 Y_{H2}= 6.269 Y_{N2}= 0.426 Y_{CH4}= 12.11 Y_{H2O}= 33.292 Y_{H2S}= 0.36

Results and Discussion

Syngas Compositions Produced from Gasifiers

Partial combustion of coal inside the gasifier produces raw syngas consisting of different gases. Some of these are re-burned again in the turbine, such as CO, H_2, and CH_4. Some are disposed off, including H_2S. Some species will withdraw heat from the system, such as N2 and water. Some gases such as CO_2 are harmful to the environment. Tables 6, 7, and 8 give the raw syngas compositions, as obtained from the above calculations, for all coal ranks, for the three studied gasifiers.

The numbers in Tables 6, 7, and 8 indicate the mole percentage of each gas component produced in the syngas by the partial combustion of coal. The mass ratio of each gas was not calculated, and it was sufficient to adopt the mole percentage values because they are more precise in expressing the gas composition since the mole mass for each gas species is different.

Table 6: Table 6: Syngas composition from entrained flow gasifier.

Gas composition	Coal rank			
	Anthracite	Bituminous	Sub bituminous	Lignite
CO %	58.792	52.958	49.304	42.926
CO_2 %	7.564	6.814	6.344	5.523
H_2 %	30.126	38.075	31.33	24.418
N_2 %	0.2	0.358	0.556	0339
CH_4 %	0	0	0	0
H_2S %	0.2	0.478	0.111	0.29
H_2O %	3.118	1.315	12.354	26.502

Table 7: Syngas composition from fluidized bed gasifier.

Gas composition	Coal rank			
	Anthracite	Bituminous	Sub bituminous	Lignite
CO %	47.121	42.33	39.533	34.446
CO_2 %	12.773	11.474	10.716	9.337
H_2 %	32.561	40.428	33.314	26.318
N_2 %	0.198	0.356	0.555	0.338
CH_4 %	4.235	3.805	3.553	3.096
H_2S %	0	0	0	0
H_2O %	3.11	1.605	12.326	26.463

Table 8: Syngas composition from fixed bed gasifier.

Gas composition	Coal rank			
	Anthracite	Bituminous	Sub bituminous	Lignite
CO %	68.047	58.79	53.706	44.978
CO_2 %	3.867	3.341	3.052	2.556
H_2 %	4.88	18.775	11.773	6.269
N_2 %	0.276	0.477	0.726	0.426
CH_4 %	18.324	15.831	14.462	12.11
H_2S %	0.276	0.636	0.145	0.365
H_2O %	4.327	2.148	16.133	33.292

As seen the main components of the syngas are the two reactive species H_2 and CO in addition to some CH_4 and CO_2. The syngas composition depends significantly, as show in Tables 6, 7, and 8, on the gasification process and the coal rank. Each gasification technology has its own gasifier design with a specific chemical reaction and operating conditions. Coals have different constituents and chemical and physical properties. All these justify dependence of syngas composition on the gasifier type and coal rank. Syngas composition depends on other factors, such as coal preparation and its particle size, coal and gas residence time in the gasifier, coal feeding procedure whether dry or slurry, heating rate, flow directions, method of mineral removal (dry ash or slag), heat generation source, and operating temperature and pressure. No one gasifier or coal type will satisfy the desired application or syngas composition and it is a matter of compromise and trade off. It is seen from the above results that the entrained flow gasifier produces a satisfactory syngas composition with varying values for different coal ranks.

The main aim of combusting syngas is the production of heat and to result in less emissions. To generate high combustion, heat the fed syngas to the gas turbine should be rich in H_2 and CO in addition to light hydrocarbons. The syngas should contain minimum or no CH_4 and sulphur in order to reduce emissions. Less sulfur means significantly lower SOx emissions than that from conventional power systems.

The composition of syngas immensely influences the emission levels. The combustion of H_2 and CO gases result in higher combustion temperature which favours thermal NOx formation. NOx can be either thermal (30%) or fuel (70%). However, such higher temperatures lead to complete combustion and hence reduces emissions of organic volatile matter which are traces of hydrocarbons in the syngas. NOx formation is a concerning issue in burning fuels whether fossil or syngas. To reduce fuel NOx, which constitutes the higher percentage of the total NOx, the nitrogen content in syngas should be small in addition to reducing the contact time between the fixed N_2 in fuel and O_2 in the combustion air. Various technologies are already available to reduce thermal NOx, e.g. flue gas recirculation (FGR) and staged combustion which reduces also fuel NOx.

Syngas combustion is greatly affected by the content of H_2 in it. The burning velocity increases with the existed amount of H_2 because the density is much less compared with that of natural gas. Also increasing the H_2 content in syngas increases the flame stability. The presence of CH_4 in syngas reduces the peak flame temperature but increases the prompt NO significantly.

The raw syngas produced from gasifiers needs a cleaning system in case used as fuel for a gas turbine in an IGCC plant. Cleaning syngas means the removal of particulate matter, metallic compounds, and other undesirable pollutants such as sulphur. The cleaning system may be pre-combustion or post-combustion. A water gas shift system may be included to enhance the H_2 content in the gas. A CO_2 capture system can be employed if desired. Therefore, IGCC plants are more environmentally cleaner than current ones especially if CO_2 capture system is adopted.

It should be realized that there are many technological problems which should be encountered for a successful IGCC technology. The most important issue is the gas turbine which is the core of a combined cycle system. The differences in the properties between syngas and NG dictate new considerations in the design of the gas turbine in an IGCC system. For instance, the lower calorific value of syngas fuels requires a significant increase in the mass flow rate of fuel supply to the gas turbine as compared with burning NG. As a result the output power will increase and this needs a different design of the turbine to allow for the increased flow rate. Also the higher content of H_2 in syngas which has a higher flame velocity may lead to difficulties in controlling the combustion mechanism. Also, syngas combustion is different from NG because of the presence of H_2 and CO which have higher adiabatic flame temperatures than CH_4. So, new issues should be looked after for a proper reliable gas turbine performance.

Cold Gas Efficiency

Table 9 exhibits the CGη and CCη for the different gasifiers and coals. Figure 6 lists some cold gas efficiencies for various gasification processes for all coal ranks. The cold gas efficiency is the ratio of fuel heat content to the syngas heat content at ambient conditions and is a measure of how efficiently fuel energy is converted into syngas energy. For the cases reported, the fixed bed is most efficient but has the disadvantage that some of the syngas energy is produced in tars. The listed efficiencies (~86%) support the rule of thumb that approximately 15% of the feedstock heating value is used to convert the feedstock to syngas.

Table 9: Coal gasification (CGη) and coal capture (CCη) efficiencies for different gasifiers and coal ranks.

Coal	Gasifier					
	Entrained flow		Fluidized bed		Fixed bed	
	(CGη)	(CCη)	(CGη)	(CCη)	(CGη)	(CCη)
	%					
Anthracite	82.22	100	84.76	97	86.92	98
Bituminous	81.72		84.23		85.88	
Sub- bituminous	80.31		82.57		84.59	
Lignite	78.32		80.83		82.66	

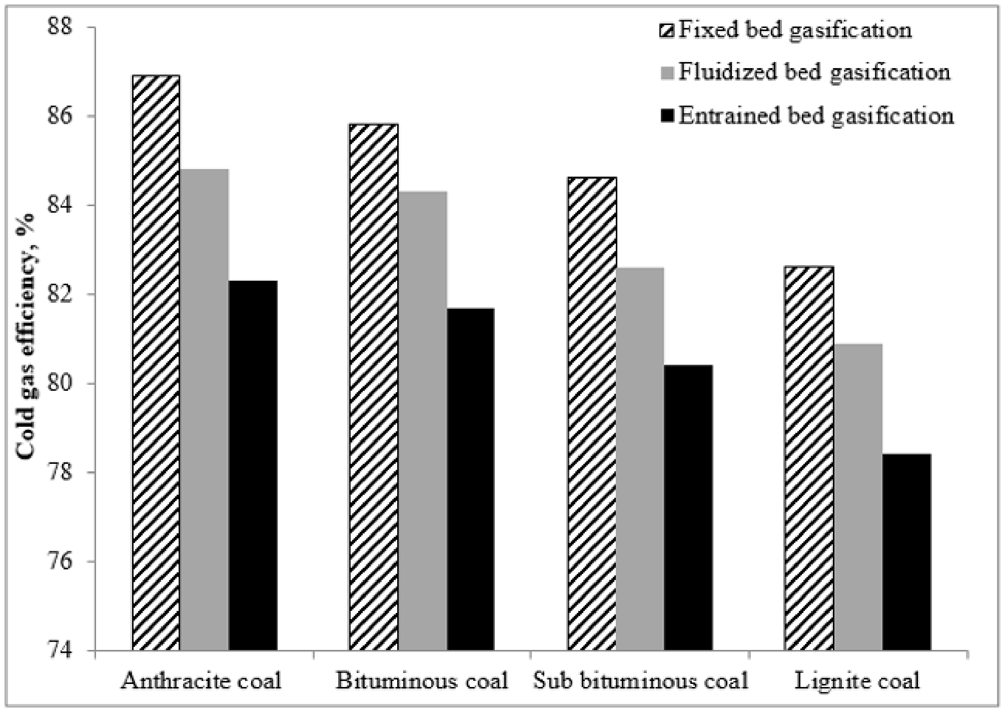

Figure 6: Cold gas efficiency, %.

The results depict that the entrained flow gasifier, for all coal ranks, is the predominant one because of its low cold gas efficiency which means low loses in coal fired because of the high temperature in the gasifier, higher carbon conversion efficiency (100%), low tar, and the low methane produced which means lower emission. The second good, for all coal types, is the fluidized bed gasifier.

Conclusions

Irrespective of new discoveries of natural gas reserves and new techniques (such as hydraulic fracturing or fracking) being developed to increase cheaper natural gas production, coal will continue to be a major energy source to produce electricity in the world, either for economic reasons or as a strategy to safeguard national energy security and independence. The conventional way of burning coal is environmentally unfriendly; therefore, it is essential that cleaner methods of utilizing coal be developed. IGCC is one of the most promising methods to generate electricity in a more efficient, environmentally friendly manner than conventional fossil fuel plants. Example step by step manual calculation procedure was conducted for one coal (bituminous).

Syngas composition depends incredibly on the gasification process and coal type. Each gasification technology has its own specific chemical reaction and operating conditions. The entrained flow gasifier satisfies most of the requirements needed for the appropriate syngas for IGCC plants, for all coals. This gasifier produces raw syngas with zero CH_4, high H_2 and CO, and low CO_2, H_2O, N_2, and H_2S.

The entrained flow gasifier is the most viable of the three because of its high carbon conversion efficiency which means low loses in coal fired and low cold gas efficiency, high temperature in the gasifier, low tar, and low methane produced resulting in low emissions, and it produces a clean gas in such a short time because of the employed high temperature. Compare this with a counter-current fixed-bed process, which uses lump coal, the heating up rate is slow with a built up of high volatiles concentration that are removed unreacted from the reactor by the syngas.

For the technology of IGCC plants to be competitive and economically feasible, their availability should be increased and the capital cost to be reduced. Achieving these, IGCC systems will be fully commercial and of increased widespread use (table 10).

Table 10.

Symbol	Description	Unit
M	Molar weight	gm/mole
ṁ	Mass flow rate	Tone per day (TPD)
T	Temperature	0C , K
HHV	High heating value	MJ/kg
LLV	Low heating value	MJ/kg
CGη	Cold gas efficiency	%
CCη	Carbon conversion efficiency	%
ΔHC	Heat of syngas	MW
FT	Fischer–Tropsch	-
IGCC	Integrated gasification combined cycle	-
ASU	Air separation unit	-
WGS	Water-gas shift	-

Conflict of Interest

The authors declare that there is no conflict of interest regarding publication of this paper.

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