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Nishant Sharma
Govt Engg College Jabalpur, nishant_24aug@rediffmail.com

Bhupendra Gupta
GEC College Gwalior, bhupendra243i@yahoo.com

Ranjeet Pratap Singh Chauhan
Department of Mechanical Engg .P.C.T., Gwl, bhanumrn@rediffmail.com

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Analysis of Exergy and Energy of Gasifier Systems for Coal-to-Fuel

[1]Nishant Sharma ,[2]Bhupendra Gupta, [3]Ranjeet Pratap Singh Chauhan

[1]Govt Engg College Jabalpur
[2]GEC College Gwalior
[3]Department of Mechanical Engg .P.C.T., Gwl
E-mail: [1] nishant_24aug@rediffmail.com , [2]bhupendra243i@yahoo.com ,[3] bhanumrn@rediffmail.com,
[4]ranjeet.singh2004@gmail.com

Abstract

The purpose of this study is to investigate the performance features of coal-to-fuel systems based on different gasification technologies. The target products are the Fischer–Tropsch synthetic crude and synthetic natural gas. Two types of entrained-flow gasifierbased coal-to-fuel systems are simulated and their performance features are discussed. One is a single-stage water quench cooling entrained-flow gasifier, and another one is a two-stage syngas cooling entrained-flow gasifier. The conservation of energy (first law of thermodynamics) and the quality of energy (second law of thermodynamics) for the systems are both investigated. The results of exergy analysis provide insights about the potential targets for technology improvement. The features of different gasifier-based coal-to-fuel systems are discussed. The results provide information about the research and development priorities in future.

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1 Introduction

As a major technology option for alternative liquid transportation fuel sources, coal to liquid (CTL) oil production has emerged in many states. In 1985, oil prices fell suddenly and remained low until recently. Interests in coal liquefaction for the production of transportation fuels declined accordingly. However, this interest has grown in the last couple of years with concerns about energy security and sustainability. While a number of factors are driving CTL projects, there are also several barriers to wide commercialization. Sasol data indicate that the production cost of CTL is generally estimated at 35–40 USD per barrel (220–250 USD/m3). In a comparison of exergy efficiencies of different gasifier-based biofuels systems, modifying the properties of the biomass feedstocks prior to gasification might also be considered as an effective way to reduce exergy This study investigated the performance features of coal-to-fuel systems.

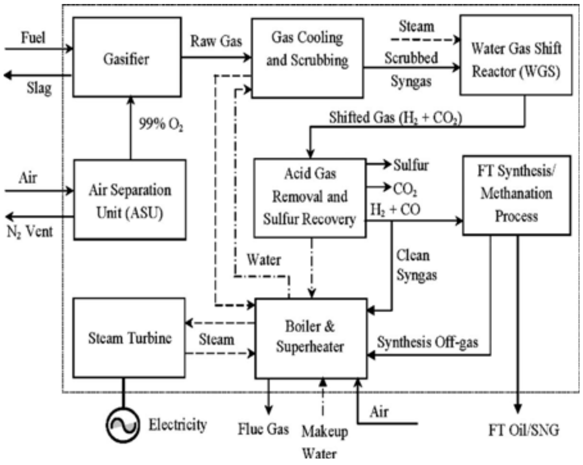

Fig. 1   for coal-to-FT oil/SNG systems

2. Design Basis

As shown in Fig. 1, main processes in a gasifier-based coal-tofuels system include gasification shift reactor, sulfur removal, fuel synthesis (FT synthesis/ methanation), and steam cycle. In a gasifier-based coal-to-fuel system, the coal and oxidant react in the gasifier to produce syngas rich in hydrogen and carbon monoxide. in this process and ready for sequestration. The removed H2S is then recovered to elemental sulfur in a sulfur recovery unit. The clean syngas with most of the H2 and CO is then sent to a synthesis process to produce FT oil or SNG.

2.1 Gasification Unit. Gasification is a process that produces syngas rich in H2 and CO from coal or other carbonaceous feedstocks. High-purity oxidant or air is fed into a gasifier to partially oxidize the feedstocks. Water or steam is used as a source of hydrolysis in gasification reactions. There are three major types of gasifiers: entrained-flow, moving-bed, and fluidized bed (10). An advantage of this type of gasifier is minimum methane production in raw syngas, which makes it suitable for being used in gasification based liquid fuels

2.1.1 Single-Stage Entrained-Flow Gasifier. Typically, slurry feed single-stage entrained-flow gasifiers have a higher operating pressure than other types of entrained-flow gasifiers, which leads to the higher syngas production capacity of gasifiers with given size. This type of gasifier has been used for conversion of heavy oils, petroleum coke, biomass, and wastes to produce power, steam, hydrogen, ammonia, or other chemicals (14).

2.1.2 Two-Stage Flow Gasifier.

In this study, a twostage entrained-flow gasifier with syngas cooler (SC) is also investigated. The design for this process is based on Wimer et al. (18) and NETL (19). In this process, coal/water slurry is injected into the gasifier with a split to process, gas cooling, water-gas

the primary and secondary stages, respectively. All the high-purity oxygen is sent to the primary stage and reacts with coal slurry fed to this stage.

Table 1 FT products distribution

CO2	0.5
C1	3.1
C2-C4	4.1
C5-C11	23.2
C12-C20	29.2
C21+	38.2

2.2 Air Separation. In this study, a cryogenic ASU is assumed for oxygen production. A cryogenic ASU mainly consists of an air compression system, cryogenic separation units, and an oxygen compression system. The air and oxygen compressors are multiple-stage air-intercooled compressors.

2.3 Syngas Conditioning and Purification. The WGS reactor is assumed to be used to adjust the syngas molar H2 /CO ratio to meet the requirement of the downstream synthesis processes. A portion of the scrubbed syngas is sent to a high temperature WGS reactor and a large part of CO is shifted to CO2. The shifted syngas is then combined with the bypassed syngas. The amount of syngas sent to the WGS is decided by the required H2 /CO ratio for FT or SNG synthesis. The shift reaction releases heat and generates high temperature shifted syngas. The high temperature

exit syngas is sent to the effluent coolers to heat boiler feed waters and generate high and low pressure steam. High pressure steam is used in the steam cycle for power generation. Low pressure steam is used for process heating. Water is condensed from the shifted gas and reused as scrubber water in the gasifier water scrubbing unit.

2.4 Sulfur Recovery Unit.. The sulfur is condensed and low pressure steam is generated. The condensed sulfur is collected as a molten liquid byproduct. The off-gas from the condensers goes to several catalytic conversion stages to convert the remaining sulfur..

2.5 FT Synthesis. The FT synthesis is a non selective process that produces a wide range of compounds containing from 1 carbon atom to 100 carbon atoms. A generalized equation describing the FT synthesis is

$$(2n + 1)\mathrm{H2} + n\mathrm{CO} \hookleftarrow \mathrm{C}n\mathrm{H}(2n+2) + n\mathrm{H2O}$$

The FT synthesis step involves competing chemical reactions that lead to a suite of desirable and undesirable products. Selectivity can be high for high molecular mass wax (25). The catalysts used in the FT process are mainly iron-based catalysts promoted with potassium, copper, and supported cobalt catalysts. The FT synthesis can produce multiple products such as a light synthetic crude oil and light olefins or heavy, waxy hydrocarbons. The synthetic crude can be refined to gasoline and diesel, by hydrocracking the waxy materials.

2.6 SNG Synthesis. In the SNG process, the primary conversion is described by the following reaction:

$$\mathrm{CO} + 3\mathrm{H2} \hookleftarrow \mathrm{CH4} + \mathrm{H2O}$$

A two-stage reactor system with internal cooling by steam generation and recycling cooled reactor effluent is assumed in this study for SNG synthesis. The recycle ratio is determined by limiting the reactor outlet temperature less than 465°C.

2.7 Steam Cycle and Power Generation. The power neutrality assumption is that the power needs for the system is balanced by the power generation from the steam turbine and no net power is generated. The steam cycle uses a fuel gas-fueled boiler and a superheater to generate steam for the turbine. High- and mediumpressure saturated steams from process cooling (mainly the WGS and FT/SNG synthesis processes)are sent to the steam cycle.

Table 2 assumptions for two different gasifiers-- coal-to-fuel

Gasifier type	Single stage flow	Two stage flow
Gasifier temp(°C)	1362	1312
Gasifier pressure(bars)	47	37
Gasifier conversion	93	93
Cooling methods(wt %)	WQ	SC
FT synthesis process		
Reactor temperature(°C)	212	212
Reactor pressure(bars)	34	22
Power Generation		
Steam Turbine bar (bars/ °C/ °C)	127/512/512	127/512/512
SNG Synthesis		
Reactor I P/T (bars/ °C)	34/465	27/470
Reactor II P/T (bars/ °C)	33/310	26/315

cannot be reached, even if the maximum recycle ratio is used in the fuel synthesis process. Therefore, the net power outputs for the two-stage SC gasifier systems are positive

3 Process Simulation Using Aspen Plus

Process simulation enables the behavior of a process to be estimated by using basic mass and energy balances, thermodynamic models, and chemical equilibrium. In this study, the different gasifier-based coal-to-fuel systems process models are developed
in Advanced System for Process Engineering Plus (Aspen Plus). Aspen Plus is an upgraded simulator based on Aspen, a deterministic steady state chemical process simulator. Aspen Plus includes an extensive thermodynamic database to support energy balance and chemical equilibrium calculations (28).

4 Process Modeling and Major Assumptions

The major inputs and assumptions of the models are listed in Table 2. For the single-stage WQ gasifier design, the hot raw gas exiting the gasifier is water-quenched. For the two-stage gasifier design, syngas coolers are used to recover sensible heat from the hot syngas by generating high pressure saturated steam.

4.1 Gasification Process Modeling. For the single-stage WQ gasifier, the coal slurry with 60 wt % dry coal flows through a slurry pump and the pressure is raised to 48 bars. The dry coal content in the slurry is specified in a calculator block in Aspen Plus. The coal slurry and oxygen are injected into the gasifier where partial oxidation of the coal takes place. The operation conditions of the gasifier have been listed in Table 2. Aspen Plus.

4.2 FT Synthesis Process Modeling

The clean syngas from the gas purification unit is combined with the recycled off-gas and then heated to 204°C by the effluent from the FT reactor. The heated gas is sent to the FT reactor, which is assumed to be a tubular fixed bed reactor.

4.3 SNG Synthesis Process Modeling.

A two-stage SNG synthesis process is assumed to be used for SNG production in this study. The cleaned syngas is first heated by the reactor effluent to 260°C. The heated gas is then mixed with steam at 352°C and 38 bars and recycled off-gas. The mixture is sent to the primary reactor of the SNG synthesis process, which is assumed to be an adiabatic fixed bed catalytic reactor. The reactor is simulated by an equilibrium reactor unit operation block in Aspen Plus.

5 Exergy Analysis

Exergy analysis is a secondary calculation typically conducted after a traditional first law system analysis is complete. Because exergy analysis is based on the total available energy of a system, including incoming fuel streams and exhaust streams, it is most useful for quantifying the environmental performance and comprehensive energy efficiency of a system

5.1 General Energy Balance Equations

The second law of thermodynamics provides a way to quantify the maximum theoretical work that could be done by a system. Exergy is destroyed by irreversibility of a process. A general exergy balance equation
for a control volume is (30)

Exergy Destruction = Exergy Input − Exergy Output

5.2 Applications to Large Control Volumes. For a steady state system, the time rate change of exergy is zero. For a control
volume, the exergy destruction is calculated as

$$Ex_{destruction} = \sum_r Q_r(1 - T_0/T_r) - W_{net} + Ex_{stream,in} - Ex_{stream,out}$$

The exergy flow of a stream is the sum of its physical exergy and chemical exergy. The total exergy flow is calculated as

$$Ex_{stream} = Ex_{ph} + Ex_{ch}$$

The physical exergy is calculated based on the property data provided by Aspen Plus. The dead state specified in Aspen Plus is T_0=298.15 K and P_0=1 atm. The chemical exergy for coal is estimated based on the correlation equation developed by Govin

- The sum of the work in and out of a control volume is calculated.
- Conservation of mass is verified to confirm that the System is operating at steady state.
- The flow rates that cross a control volume are identified And calculated.

The energy efficiency for the overall system is calculated as

$$\square = \frac{E_{fuel} + W_{net}}{E_{coal}}$$

The overall system exergy efficiency is calculated as

$$\psi = \frac{Ex_{fuel} + W_{net}}{Ex_{coal}}$$

Based on the above equations, the energy and exergy efficiencies for each system are calculated.

6 Results and Analysis

Table 3 Major simulation results for two different gasifiers based coal-to-fuel systems

	Coal to SNG oil		Coal to FT oil	
	Single stage WQ gasifier	Single stage WQ gasifier	Single stage WQ gasifier	Two stage SC gasifier
POWER				
Steam turbine (MW)	232	256	167	231
Acid remove (MW)	-7	-8	-6	-9
ASU (MW)	-131	-117	-146	-119
Other power consumption (MW)	-63	-105	-31	-42
Net power output	0	32	0	13
Total parasitic load(MW)	-231	-245	-162	-219
CONSUMABLES				
Water consumption (gpm)	1786	2132	2200	2643
O2 feed (tons/d)	8265	7423	8265	7423
Coal fed (tons/d)	11200	10344	11200	10344
PRODUCTS				
EXERGY EFFICIEN				

CY (%)	47	49	46	52
SNG(m3/h)	142	142	152	148
Energy efficiency (%)	39	43	46	54

The main simulation results are listed in Table 3. boiler. A detailed cost analysis will be conducted in future work.

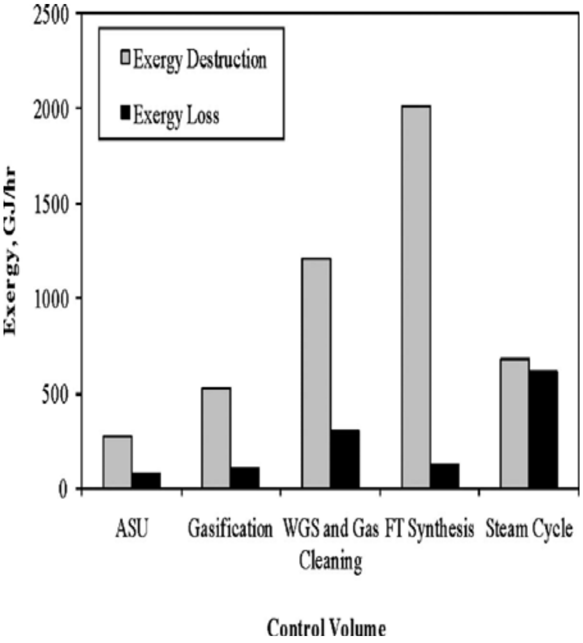

Fig. 2 Exergy analysis results of a two-stage SC gasifier-based coal-to-FT oil system

The purpose of the exergy analysis is also to identify the key control volumes with significant exergy destruction and exergy loss in a system. The two-stage SC gasifier-based coal-to-FT oil system was taken as an example for the detailed exergy destruction and losses analysis. The results are depicted in Fig. 2.

7 Conclusions

The specific conclusions are as follows.

1.Single-stage WQ gasifier-based systems have lower water consumption than two-stage SC gasifier systems. Comparing to the WQ design, the SC design increases the consumption of the boiler feed water for steam generation and thus increases the makeup water consumption of the steam cycle.

2.Exergy losses analysis showed steam cycle and WGS, and gas cleaning processes have larger exergy losses than other processes.

3. The SNG system has higher energy and exergy efficiencies than the FT oil system because of higher conversion efficiency of SNG synthesis, lower power consumption, and less heat loss for product cooling.

Nomenclature

$Ex_{destruction}$ = exergy destruction of a control volume
$Ex_{i,j}$ = exergy flow of stream i, i=fuel, coal, or stream, and j=in or out
E_i = energy flow of stream i, i=fuel or coal
In = inlet
Out = outlet
ph = physical
ch = chemical
Q_r = heat transfer rate from an energy reservoir r
T_0 = environment temperature
T_r = temperature of heat source r
W_{net} = net work produced by a control volume
□ = energy efficiency
Ψ= exergy efficiency

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