



# Modeling, thermodynamic and techno-economic analysis of coal-to-liquids process with different entrained flow coal gasifiers

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## HIGHLIGHTS

- Modeling of coal-to-liquids (CTL) process with different entrained flow gasifiers was conducted.
- Thermodynamic analysis of CTL process was presented.
- Locations and magnitudes of exergy inefficiencies were identified and quantified.
- Techno-economic and CO<sub>2</sub> emissions analysis of CTL process were conducted.

## ARTICLE INFO

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## ABSTRACT

For the coal-to-liquids (CTL) plant, the most important unit is gasification, which determines the composition of the crude syngas, and affects CO<sub>2</sub> emissions and investment of the CTL process. This paper conducts a detailed plant-wide modeling of CTL process with different entrained flow gasifiers. The model is compared with the literature data. Three cases of CTL process with different entrained flow gasifiers (GSP, Shell and Texaco) are researched through thermodynamic, techno-economic and CO<sub>2</sub> emissions analysis. Case GSP represents the CTL process with GSP gasifier, Case Shell represents that with Shell gasifier, and Case Texaco represents that with Texaco gasifier. For a typical CTL process, Case GSP can produce FT liquids of 277.49 t/h, Case Shell can produce 246.25 t/h, and Case Texaco can provide 232.93 t/h. The energy efficiencies of Case GSP, Shell and Texaco are 50.85%, 48.18% and 41.09%, respectively. The exergy efficiencies are 49.89%, 47.20% and 40.44%, respectively. The exergy inefficiencies of the subsystem are quantified. The economic performance and CO<sub>2</sub> emissions of the three cases are also discussed.

## 1. Introduction

The energy reserve in China is rich in coal, while scarcity in oil and gas. The proven reserves of coal in China are  $114.5 \times 10^9$  t, and in 2015 the percentages of energy production from coal, oil, and natural gas are 78.2%, 9.2%, and 5.3%, respectively [1]. In a long time, coal will be the dominant energy resource in China. As shown in Fig. 1, the consumption of gasoline and diesel in China has been growing rapidly [1]. The oil consumption is kept increasing, and more than half of oil is imported from abroad, so the development of alternative energy resources is required. The coal-to-liquids (CTL) process can produce diesel and gasoline from coal. The capacity of the biggest CTL plant is 4.0 Mt/y oil in

China [2], and the total capacity will grow continuously to 13 Mt/y by 2020 [3].

Gasifiers vary in cold gas efficiency, cost, processing capacity and adaptability of coal type, and this makes a big difference in the whole CTL process. There are mainly three types of gasifiers based on the solid feedstock movement, i.e., fixed bed, fluidized bed and entrained flow gasifiers. For the entrained flow gasifiers, there are two feeding options, slurry feeding and dry feeding. Recent studies on the CTL process with different gasifiers is shown in Table 1. Various of gasifiers are used (Shell, Texaco, BGL, etc.), and most studies focus on the plant configuration (liquid-only or co-production [4–8]), the integration with CCS [4–13] and hybrid feedstock (coal/biomass/natural gas [9–11,14–23]).

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Nomenclature		<i>TCI</i>	total capital investment
<i>Abbreviations</i>		<i>WGS</i>	water gas shift
<i>AGR</i>	acid gas removal	<i>WWT</i>	wastewater treatment
<i>ASU</i>	air separation unit	<i>Notations</i>	
<i>ATR</i>	autothermal reformer	<i>a, b, c, d</i>	the coefficients of specific heat capacity
<i>BEOP</i>	break-even oil price	<i>C</i>	cost
<i>BFW</i>	boiler feed water	<i>c<sub>p</sub></i>	the specific heat capacity (kJ/kg K)
<i>BOI</i>	balance of indirect costs	<i>d<sub>p</sub></i>	the diameter of the coal particle
<i>BOP</i>	balance of plant costs	<i>E<sub>x</sub></i>	Exergy (kJ/kg)
<i>BTL</i>	biomass-to-liquids	<i>H</i>	Enthalpy (kJ/kg)
<i>CBGTL</i>	coal, biomass, and natural gas to liquids	<i>n</i>	the number of carbon atoms in the hydrocarbon molecules
<i>CBTL</i>	coal biomass to liquids	<i>P</i>	Pressure (kPa)
<i>CCP</i>	combined cycle power plant	<i>S</i>	Entropy (kJ/kg K)
<i>CCS</i>	CO <sub>2</sub> capture and storage	<i>S<sub>1</sub>, S<sub>2</sub></i>	the production capacity of the benchmark project and the planning project
<i>CEPCI</i>	Chemical Engineering Plant Cost Index	<i>T</i>	Temperature (K)
<i>CG</i>	coal gasification	<i>t<sub>n</sub></i>	number of trains
<i>CoP</i>	ConocoPhillips	<i>x<sub>i</sub></i>	the mass fraction of component <i>i</i>
<i>CTL</i>	coal-to-liquids	<i>Y</i>	yield
<i>EG</i>	ethylene glycol	<i>y<sub>ineff</sub></i>	the ratio of the exergy inefficiencies to the total exergy inefficiencies
<i>FCI</i>	fixed capital investment	<i>Z</i>	the coefficient which depends on the concentration of CO and CO <sub>2</sub>
<i>FG</i>	fuel gas	[CO]	the concentration of CO
<i>FT</i>	Fischer-Tropsch	[CO <sub>2</sub> ]	the concentration of CO <sub>2</sub>
<i>FTL</i>	FT liquids	<i>Greek symbols</i>	
<i>GE-Texaco</i>	Texaco	<i>η<sub>x</sub></i>	exergy efficiency (%)
<i>GT</i>	gas turbine	<i>Φ</i>	the coefficient which depends on the diameter of the coal particle
<i>GTL</i>	natural gas to liquids	<i>Subscripts and superscripts</i>	
<i>HP</i>	high pressure	0	reference state
<i>HRS</i>	heat recovery steam generator	daf	dry, ash free
<i>IP</i>	intermediate pressure	dev	devolatilization
<i>LACCR</i>	the levelized annual capital charge rate	e	electricity
<i>LFG</i>	light fuel gas	ex	exergy
<i>LHV</i>	lower heating values	in	input
<i>LP</i>	low pressure	ind	indirect
<i>LRC</i>	low-rank coal	ineff	exergy inefficiencies
<i>LTFT</i>	low-temperature FT	out	output
<i>MDEA</i>	methyldiethanolamine	ph	physical
<i>MHX</i>	main heat exchanger	prod	product
<i>NG</i>	natural gas	th	thermal
<i>O&amp;M</i>	operating and maintenance	VM	volatile matter
<i>OTL</i>	oil-to-liquid fuels		
<i>PSA</i>	pressure swing adsorption		
<i>SCOT</i>	Shell Claus off-gas treating		
<i>Siemens-GSP</i>	GSP		
<i>sf</i>	the scale factor		
<i>ST</i>	steam turbine		
<i>STL</i>	shale-to-liquids		
<i>SWS</i>	sour water stripper		

Only a few authors considered the effect of gasifier type. The CTL plants in China mainly use three types of gasifiers, i.e., slurry gasifiers, dry powder gasifiers, and fixed bed gasifiers [24]. As the entrained flow gasifiers have four main advantages: (1) the ability to utilize any type of coal, (2) high coal throughput capacity particularly at high pressures, (3) product gas is free of tars, and (4) high carbon utilization due to high reaction rates, this study focuses on the entrained flow gasifiers, and three types of entrained flow gasifiers (GSP, Shell and Texaco) are systematically investigated to assess their performance in the CTL process.

Exergy is defined as the maximum theoretical work obtainable from a system compared with the ambient environment. It is used to assess thermodynamic inefficiencies in the system by considering the magnitudes, locations, and types of exergy inefficiencies [27]. The exergy

analysis methodology has been applied in the coal gasification (CG) [28–30], biomass gasification [31–36], CTL process [37], GTL process [38], and BTL process [39–42]. Gräbner and Meyer [28] evaluated the gasification processes in terms of cold gas efficiency, syngas yield and exergy efficiency. CoP and Shell exhibited the highest exergy efficiencies for Pittsburgh #8 coal while Siemens (GSP) offered the highest efficiency for the South African coal. Liszka et al. [29] proposed a hydrogen production process through co-gasification of biomass and coal with CO<sub>2</sub> capture. The overall exergy efficiency of the coal-to-hydrogen system was 57%, and the highest exergy losses took place in the gasifier. Seyitoglu et al. [30] studied an integrated coal gasification system for hydrogen production and power generation, and the overall energy and exergy efficiencies of the entire system was 41% and 36.5%, respectively. Ptasiński et al. [31] used idealized gasifier model to

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