



# Analysis and assessment of a hydrogen production plant consisting of coal gasification, thermochemical water decomposition and hydrogen compression systems

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## ABSTRACT

A novel hydrogen production plant is proposed, including a thermochemical water decomposition cycle, a pressurized entrained flow gasifier, a water gas shift membrane reactor, a cryogenic air separation unit, a hydrogen-fueled combined cycle for power production and a hydrogen compression system. The syngas produced by the pressurized entrained flow gasifier undergoes the shift reaction in the water gas shift membrane reactor. The stripping of hydrogen is done simultaneously with the shift reaction in the water gas shift membrane reactor to capture more hydrogen and increase the shift reaction conversion percentage. The remaining syngas is combusted in the Brayton cycle and power is produced through Brayton cycle gas turbine. The hot exhausts exiting the Brayton cycle gas turbine goes to the heat recovery steam generation unit where steam is produced. The generated steam goes to the copper-chlorine cycle to produce hydrogen. Part of the power generated by the Brayton cycle is used for the electrolysis reactor in the copper-chlorine cycle. Then, a small part of the hydrogen produced passes to the combined cycle to overcome the needed work rate by the components in the plant. The remaining larger portion of the hydrogen produced goes to the compression system to compress hydrogen to 700 bar for storage. The hydrogen production plant is developed and modeled in the Aspen Plus software package. Energy and exergy analyses are performed on the hydrogen production integrated system. The overall energy and exergy efficiencies of the proposed hydrogen production plant are found to be 51.3% and 47.6% respectively.

## 1. Introduction

People are gradually depleting the world's fossil fuels resources, forcing humanity to find alternative sources of energy to meet the continuously rising demands for energy. Recent reports by the International Energy Agency predict an increase in global energy demand of 50% by 2030 [1]. Concerns about the limited nature of the fossil fuels have resulted in extensive research and development on alternative sources of energy and on how to use currently available fossil fuels more efficiently. Many methods are used today to increase the efficiency of energy production from fossil fuels; one of these methods is to run the power plants at a constant rate and at full capacity all the time, another approach is the integration of power systems. Running power plants at full capacity is not possible due to the fluctuating nature of the energy demands during night and day, summer and winter. However, the successful use of energy storage systems can make that possible. Hydrogen has the advantage of being both energy

storage medium and an energy carrier [2], meaning that running power plants at full capacity and storing the excess energy in hydrogen will result in more efficient use of the available fossil fuels. Muradov and Veziroglu [3] analyzed the main methods for hydrogen production from fossil fuels as a green path for fossil-based hydrogen production, one of these methods is water electrolysis, and another promising hydrogen production process is the thermochemical copper-chlorine cycle. An advantage of the thermochemical hydrogen production cycle is that it directly produces hydrogen from heat without the intermediate step of heat to electricity, which is vital for water electrolysis.

A number of researchers have proposed various integrations of gasification of coal with other systems, such as [4,5] where they have utilized an IGCC system integrated with a Cu-Cl cycle, which provides the oxygen to the coal gasifier. Other researchers looked into replacing the oxygen blown gasifier with an air blown gasifier, and they have investigated the IGCC system performance under each [7]. They have found out that the air blown gasifier perform better than the oxygen

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Nomenclature	
COP	coefficient of performance
$\dot{E}_x$	exergy rate (kW)
ex	specific exergy (kJ/kg)
h	specific enthalpy (kJ/kg)
HHV	higher heating value (kJ/kg)
HV	heating value (kJ/kg)
LHV	lower heating value (kJ/kg)
$\dot{m}$	mass flow rate (kg/s)
P	pressure (kPa)
$\dot{Q}$	heat rate (kW)
R	universal gas constant (kJ/mol.K)
s	specific entropy (kJ/kg.K)
S	sulfur content in coal (see Eq. (37))
T	temperature (°C)
$\dot{W}$	work rate (kW)
x	Mole fraction of constituent j in the flow (moles of J/moles of the total flow)
<i>Greek letters</i>	
$\beta$	Coal parameter calculated using Eq. (38)
$\eta$	energy efficiency
$\psi$	exergy efficiency
$\omega$	moisture content in coal
<i>Subscripts</i>	
BrC	Brayton cycle
CASU	cryogenic air separation unit
ch	chemical
Cu-Cl	copper-chlorine cycle
coal	coal
d	destruction
e	electrical
fg	phase change between liquid and gas
gen	generation
GT	gas turbine
G&U	gasifier and utilities
HFCC	hydrogen fueled combined cycle
H <sub>2</sub>	hydrogen
HCS	hydrogen compression system
is	isentropic
in	input (flowing into the system boundary)
i	state point named i
j	constituent name in the flow
net	net result
ov	overall
out	output (flowing out of the system boundary)
o	at standard conditions
$\dot{Q}$	heat flow rate
RC	Rankine cycle
ST	steam turbine
s	the boundary where heat transfer takes
W	work
WGSMR	water gas shift membrane reactor
<i>Superscripts</i>	
coal	coal
o	at standard conditions
<i>Acronyms</i>	
BrC	Brayton cycle
CASU	cryogenic air separation unit
Cu-Cl	copper-chlorine cycle
GFEMA	Gibbs free energy minimization approach
HRSG	heat recovery steam generator
HFCC	hydrogen fueled combined cycle
HCS	hydrogen compression system
IGCC	integrated gasification combined cycle
O/C	oxygen content in the coal divided by the carbon content in the coal
RC	Rankin cycle
WGSMR	water gas shift membrane reactor
<i>Aspen Plus terms</i>	
Rstoic	Stoichiometric reactor
Cisolid	for homogeneous solids that have a defined molecular weight, with the option of entering the particle size distribution
NC	nonconventional solid (for heterogeneous solids that have no defined molecular weight) with the option of entering the particle size distribution

blown gasifier, however the results were specific for the specific air separation technology considered. The performance of an IGCC system was compared for two different cases of output product in Ref. [8]. The first case, the IGCC system was producing only electrical power, while the second case the IGCC system was producing only hydrogen. The results presented by Gnanapragasam et al. [8] indicated that the hydrogen production system appears to be advantageous over the IGCC system based on their selected analysis method. Rather than having an IGCC system with a single product, Seyitoglu et al. [9] proposed and analyzed the performance of a trigeneration IGCC system, and they proposed system is proposed to produce hydrogen, power and Fischer-Tropsch synthesis products. The research outcomes of Refs. [8,9] concluded that multigenerational IGCC systems were able to achieve higher energy and exergy efficiency compared to single generation systems.

Further research was focused on optimizing the gasification process through the introducing the thermal energy for renewable energy sources, where solar energy was utilized in a coal gasification based multi-generational system [10]. However, other investigated the performance of an IGCC system where a dual chemical looping occurred

simultaneously with gasification, where the effect of several factors were investigated such as oxygen, steam and CaO flow to coal ratios [11]. The performance of an IGCC system for three different types of fuel feed, which are coal, biomass and a combination of both [12]. However, the combinations introduced in [12] were limited to couple of combined flows, which resulted in a very limited results that derived from specific combinations. In order to have a more flexible models to investigate the effect of wide range of fuel compositions, Cohce et al. [13] proposed an ideal gasification model in Aspen Plus, which was able to predict the syngas composition with an acceptable accuracy based on the authors.

Researchers have proposed various integrations of gasification of coal [5–12,16], biomass [13], or the combination of coal and biomass [12] with other systems such as a solar power tower [10], or with a Fischer-Tropsch unit [9]. Others have integrated the gasification system with a dual chemical looping process, namely chemical looping air separation and water gas shift with calcium looping CO<sub>2</sub> absorption [11]. The production of hydrogen from coals is primarily achieved through gasification, which produces syngas. Syngas is further treated

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