



Development of an integrated system for electricity and hydrogen production from coal and water utilizing a novel chemical hydrogen storage technology



Maan Al-Zareer*, Ibrahim Dincer, Marc A. Rosen

Clean Energy Research Laboratory, Faculty of Engineering and Applied Science, University of Ontario Institute of Technology, 2000 Simcoe Street North, Oshawa, Ontario L1H 7K4, Canada

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ABSTRACT

A coal gasification-based integrated system is proposed to produce electrical power and hydrogen. The hydrogen produced is stored in a chemical storage medium, which is ammonia. The integrated system contains a water gas shift membrane reactor, a hybrid thermochemical water decomposition cycle based on the chemical couple copper and chlorine and a multistage ammonia production system. A hydrogen fueled supporting combined cycle is used to meet the electrical requirement of the integrated system. Coal is gasified, and the resulting syngas is water shifted in a membrane reactor, which produces hydrogen. The remaining syngas is combusted to generate power through a gas turbine, and the turbine hot exhaust is used to provide the required thermal energy of the water decomposition cycle. The hydrogen outputs from the coal gasification and the water decomposition cycle are fed to the ammonia production system and the supporting combined cycle. The ammonia production system contains multiple stages to achieve a high conversion percentage of hydrogen. The nitrogen fed to the ammonia reactor is provided by the cryogenic air separation unit, which also provides oxygen to the gasifier. The proposed system is simulated with the process simulation software Aspen Plus. The system performance is evaluated through energy and exergy efficiencies. The integrated system is found to have an energy efficiency of 48.7% and an exergy efficiency of 48.4%. The system is capable of producing 0.18 kg/s of hydrogen and 1.2 MW of power per 1.5 kg/s of coal.

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1. Introduction

The world requires many services and goods, such as space heating, space cooling, chemicals and electricity. These services are typically satisfied by energy and, based on one of the latest reports by the International Energy Agency, the global energy demand will increase by up to 50% in the next 14 years [1]. Most (78%) of the world energy demand is obtained from fossil fuels, one of the main contributors to global warming [1].

Fossil fuels are considered finite in nature and not renewable as well as not sustainable. The current energy situation in the world is fostering research and development to make the use of available sources of energy more efficient. One of the causes for energy losses is the difficulty in matching energy generation and energy demand temporally. An energy storage can help in matching these by storing excess energy and until it is required [2]. Hydrogen is a clean energy carrier (if produced from clean energy sources) and can serve as an energy storage medium [3]. Although hydrogen has one of the highest specific energies (energy per unit mass), it has a very low mass density. The low mass density of

hydrogen makes storing it for industrial applications at normal ambient pressure and temperature an impractical task.

Many technologies are available to store hydrogen. It can be stored as a compressed gas, which involves compressing hydrogen to a very high pressure, around 700 bar, and then cooling it to ambient conditions. For example, Ezzat and Dincer [4] proposed a vehicle system that runs on compressed hydrogen stored in a tank at 700 bar. Another storage process involves hydrogen cryogenic liquefaction, with hydrogen stored in the liquid phase. However, the former process requires a storage tank of high strength to withstand the pressure and the latter high insulation to prevent the hydrogen from evaporating. In both cases, hydrogen can leak, leading to an explosion risk.

Another hydrogen storage process, that addresses the previously mentioned problems while maintaining a carbon-free fuel, is through ammonia (NH₃), i.e., chemical energy storage. Ammonia can be produced from hydrogen and nitrogen. Ammonia has a lower heating value nearly 70% of that of hydrogen (on a mass basis). The stored hydrogen in ammonia can be recovered by ammonia electrolysis, which theoretically requires only 5% of the electrical energy used in water electrolysis per gram of produced hydrogen [5]. At ambient pressure, ammonia is a liquid at temperatures between −33.3 °C and −77.7 °C, while hydrogen is a liquid at temperatures below −252.8 °C. Storing

* Corresponding author.

E-mail addresses: maan.al-zareer@uoit.ca (M. Al-Zareer), ibrahim.dincer@uoit.ca (I. Dincer), marc.rosen@uoit.ca (M.A. Rosen).

Nomenclature

c_p	specific heat at constant pressure (kJ/kg K)
ex	specific exergy (kJ/kg)
$\dot{E}x$	exergy rate (kW)
h	specific enthalpy (kJ/kg)
LHV	lower heating value (kJ/mol)
\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)
T	temperature ($^{\circ}$ C)
\dot{W}	work rate (kW)
x	mass vapor fraction (kg_{vapor}/kg_{total})

Greek letters

η	energy efficiency
ψ	exergy efficiency

Subscripts

airC	air compressor
Cu-Cl	copper-chlorine
CASU	cryogenic air separation unit
d	destruction
e	electrical
f	formation
gen	generation
HFCC	hydrogen fueled combined cycle
HRRC	heat recovery Rankine cycle
is	isentropic
in	input (flowing into system boundary)
max	maximum
MsAP	multistage ammonia production
net	net result
ov	overall
out	output (flowing out of system boundary)
o	reference environment conditions
\dot{Q}	heat flow rate
ST	steam turbine
SCRC	steam circuit Rankine cycle
SFBC	syngas fueled Brayton cycle
bs	boundary where heat transfer occurs
W	work
WGSMR	water gas shift membrane reactor
@P&T	at pressure P and temperature T

Acronyms

CASU	Cryogenic air separation unit
HFCC	Hydrogen fueled combined cycle
HRRC	Heat recovery Rankine cycle
MsAP	Multistage ammonia production
SCRC	Steam circuit Rankine cycle
SFBC	Syngas fueled Brayton cycle
WGSMR	Water gas shift membrane reactor

Hydrogen can be converted to electricity through fuel cells, to thermal energy by combustion, and to other chemical materials that have a wide variety of uses. The only product of oxidizing hydrogen is water (H_2O) [6].

Hydrogen can be produced from fossil fuels through various technologies, such as (a) steam methane reforming, (b) coal gasification, and (c) decomposing water through electrolysis. Muradov and Veziroglu [7] analyzed methods for producing hydrogen from fossil fuels and identified the hybrid thermochemical decomposition of water as a promising technology. Coal gasification can be integrated with a combined cycle to form an integrated gasification combined cycle (IGCC) [8–15]. It has been reported that 18% of the hydrogen produced worldwide is from coal [16]. Various studies propose integrating IGCC with other systems and cycles for increasing efficiency [9,13,14,17–22]. One integration involves combining coal and biomass as the gasifier fuel [21], while IGCC has also been integrate with a solar power tower [19] and the Fischer-Tropsch process [9]. El-Emam et al. [23] proposed a system integrating a coal gasifier and a solid oxide fuel cell and found the system energy and exergy efficiencies to be 38.1% and 36.7%, respectively. Al-Zareer et al. [15] developed and analyzed an IGCC system integrated with a water gas shift membrane reactor and a direct H_2S decomposition reactor. In that work, a supercritical water Rankine cycle produces electrical power from the thermal energy of the gas turbine exhaust with energy and exergy efficiencies of 39% and 44%, respectively. Other studies have focused on the coal gasifier, e.g., Al-Zareer et al. [24] developed two gasification models in Aspen Plus, one based on the coal gasification reaction kinetics of a specific coal type (Illinois No. 6) and the other based on a Gibbs free energy based model. Al-Zareer et al. [24] found that the Gibbs free energy model exhibits a maximum difference from experimental results of 6.5% in the mole fraction of hydrogen in the resulting syngas.

Current interest in hydrogen production through hybrid thermochemical water decomposition has led researchers to integrate it with other energy systems [17,25–28]. One of the few studies integrating IGCC with thermochemical water decomposition is by Aghahosseini et al. [17], who analyzed an IGCC system integrated with a thermochemical water decomposition cycle for trigeneration of hydrogen, steam, and electricity. The gasifier in [17] is oxygen based, and in the integrated system 60% of the thermal energy received by the water decomposition cycle is from the IGCC plant. Aghahosseini et al. [17] identified significant improvements in the overall hydrogen, steam and electricity outputs in the integrated system compared to standalone systems. The thermochemical water decomposition cycle used in the integrated system is based on the chemical couple copper and chlorine. The cycle has a number of variations depending on the number and types of main steps [29]. Orhan et al. [27,30] performed energy and exergy analyses of several configurations of the Cu-Cl cycle. The Cu-Cl cycle has also been analyzed with exergoeconomic analysis, an exergy-based economic method, and based on other evaluation criteria [17,25–28,30–52]. A small number of researchers propose integrated systems that combined the Cu-Cl cycle, coal-based systems and other technologies for hydrogen production or multigenerational systems [26,45,51]. More work is needed on integrating the Cu-Cl cycle with other systems to increase the overall efficiency of the hydrogen production process and identify more efficient methods for delivering thermal energy to the cycle reactors. This includes work on preparing the produced hydrogen for storage.

The aim of this paper is to develop and analyze the performance of a coal-based integrated system that contains a Cu-Cl cycle for generation of hydrogen and electrical power. The Cu-Cl cycle in the integrated system is based on the four-step cycle that is currently being developed in the Clean Energy Research Laboratory at the University of Ontario Institute of Technology, and is a hybrid thermochemical water decomposition cycle, i.e., one requiring both electrical energy and thermal energy. The integrated system provides thermal energy to the Cu-Cl cycle reactors via a steam circuit. The proposed design of the steam circuit includes devices to reduce energy losses and to produce electrical power to satisfy

hydrogen in ammonia has some advantages; the hydrogen can be recovered by reacting the ammonia electrically through an ammonia electrolyzer.

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