SIMULATION AND OPTIMIZATION OF ETHANOL AUTOTHERMAL REFORMER FOR FUEL CELL APPLICATIONS

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ABSTRACT

Fuel cell application from hydrogen was one of alternative energy that being studied and widely accepted in industry. This case study focused on optimization of hydrogen production for fuel cell applications. In this case study, ethanol was chosen as a raw material and with autothermal reforming as a process of produce hydrogen. Using a commercial dynamic flow sheeting software, HYSYS 3.2, the process of hydrogen production was successfully simulated. In this research, fuel processor consists of an autothermal reactor, three water gas shift reactors and a preferential oxidation reactor was successfully developed. The purpose of this case study is to identify the effect of various operating parameters such as air-to-fuel (A/F) ratio and steam-to-fuel (S/F) ratio to get the optimum hydrogen production while made carbon monoxide lower than 10 ppm. From the results, an optimum A/F and S/F ratio are 5.5 and 1.5, respectively to produce 34 % of hydrogen and 10.055 ppm of CO. Under these optimum conditions, 83.6% of fuel processor efficiency was achieved.

ABSTRAK

Penggunaan sel bahan api daripada hidrogen merupakan salah satu tenaga yang masih dikaji dan diterima dalam kebanyakan industri. Kajian ini memfokuskan tentang pengeluaran hidrogen untuk penggunaan sel bahan api secara dinamik. Dalam kajian ini, etanol dipilih sebagai bahan mentah dan pembentukan autoterma (*auto thermal reforming*) merupakan proses untuk menghasilkan hidrogen. Dengan menggunakan perisian ‘HYSYS 3.2, proses pengeluaran hidrogen ini berjaya dilakukan secara simulasi. Dalam kajian ini, pemproses minyak mengandungi reaktor autoterma,, tiga reaktor anjakan air gas dan reaktor pilihan pengoksidaan telah berjaya dihasilkan. Kajian ini bertujuan untuk mengenalpasti kesan pengandelaian parameter yang berlainan seperti ratio udara-ke-minyak (A/F) dan ratio stim-ke-minyak (S/F) untuk mendapatkan pengeluaran hydrogen yang optimum sementara CO dihasilkan rendah dari 10 ppm. Daripada keputusan ujikaji, nilai ratio A/F dan S/F yang optima adalah 5.5 dan 1.5 masing-masing. Dengan ratio tersebut,34% hydrogen dan 10.055 ppm CO dapat dihasilkan. Dibawah keadaan pengoptimaan ini, sebanyak 83.6 % kecekapan pemproses minyak didapati.

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LIST OF SYMBOLS

A	Heat transfer area
a	Parameter, cubic equation of state
b	Parameter, cubic equation of state
C	Concentration
F	Volumetric flow rate
g	Local acceleration of gravity
H	Molar or specific enthalpy
h	Step size
k	Kinetic energy
$\dot{m}$	Mass flow rate
MW	Molecular weight
N_m	Number of independent variables
N_{om}	Number of manipulated variables with no steady state effect
N_{oy}	Number of variables that need to be controlled from N_m
N_{ss}	Number of variables needed to be specified
P	Absolute pressure
P_o	Reference pressure
P_{ci}	Critical pressure, species i
P_{ri}	Reduced pressure, species i
Q	Heat
Qr	Heat generated by reaction
R	Universal gas constant
r	Rate of reaction
t	Time
u	Internal energy
V	Volume

Y	Process Variable

Greek letters

α	Function, cubic equation of state
ε	Error
μ	Viscosity
ρ	Density
φ	Potential energy
ω	Acentric factor

Abbreviations

ATR	Auto thermal reforming
ca.	at approximate
CO	Carbon Monoxide
CO_2	Carbon Dioxide
et al.	et alias: and others
etc.	et cetera
H_2	Hydrogen
HTS	High Temperature Shift
LTS	Lower Temperature Shift
PROX	Preferential Oxidation
MTS	Medium Temperature Shift
WGS	Water Gas Shift

CHAPTER I

INTRODUCTION

1.1 Background Research

Hydrogen was expected to become an important energy carrier for sustainable energy consumption with a significantly reduced impact on the environment. Hydrogen's benefit and disadvantages differ from the fossil fuels common place in advanced energy utilizing society. It is because characteristics of hydrogen that cheap, easy to obtain, high efficiency, virtually silent operation and less pollutant emissions. (Fuel cell store website, 2006)

From that perspective, researcher over the world tries to make use the hydrogen as an alternative energy by converting into fuel cell. Hydrogen as fuel cell technology currently needed in large quantities, and is projected to be the fuel of choice for a number of advanced technologies that are being pursued. Fuel cell will supply the energy that a global society requires to support the growing number of people that demanding on fuel cell technology using hydrogen. (Fuel cell store website, 2006)

For that purpose, some fossil fuels which have high hydrogen to oxygen ratio were the best candidates to produce hydrogen. The more hydrogen present and the fewer extraneous compounds was the idea to get it. One of the methods which commonly being used was the steam reforming. Other established methods include partial oxidation of residual oil, coal gasification, water electrolysis and etc. The new technologies such as high-temperature electrolysis of steam, thermal cracking of natural gas, thermo chemical water splitting, solar photovoltaic water electrolysis, and plasma decomposition of water is still investigated its efficiency. These technologies can be classified as thermal, thermo chemical, electrochemical, photochemical, and plasma chemical methods. (Fuel cell store website, 2006)

Seven common fuels are the postulated hydrogen sources studied in this work alcohol, natural gas, gasoline, diesel fuel, aviation jet fuel, and hydrogen itself. Among the bio-fuel candidates for carriers of hydrogen, ethanol is of particular interest because its low toxicity, low production costs, the fact that is a relative clean fuel in terms of composition, relatively high hydrogen content and availability and ease of handling. Hydrogen can be obtained directly from ethanol by two main processes; partial oxidation and steam reforming. (Fuel cell store website, 2006)

1.2 Problem Statement

In reality, chemical plants are never truly at steady state. Feed and environmental disturbances, heat exchanger fouling, and catalytic degradation continuously upset the conditions of a smooth running process. Optimization simulation can help researcher to make better design, optimize, and operate process or refining plant. In this research, ethanol is the main focus to study the steady state behaviour. Furthermore, the optimization is the main case study that will make more yield selectivity hydrogen. The important of this study is to identify design parameters and also to estimate fuel processor efficiency.

1.3 Research Objectives

The main objective of this research is to simulate and optimize the hydrogen production plant for fuel cell application using ethanol via autothermal reformer.

1.4 Scope of Study

To achieve above objective, several scopes has be drawn:

i. Base case simulation development
By using Aspen HYSYS 3.2, hydrogen production simulation plant was being developed with data from Akande et al. (2005)

ii. Base case simulation validation
From base case simulation that being developed with Aspen HYSYS 3.2, it was validated using theoretically data from total reactions stoichiometry coefficient.

iii. ATR optimization
ATR was optimizing by optimized the air feed molar that enter the ATR while monitoring the production of hydrogen and carbon monoxide (CO) in a certain range of temperature.

iv. Heat integration
This system is used to increase the efficiency of the plant by using heat exchanger to cool down the ATR vapour out with the hot stream from the feed.

v. Carbon monoxide clean up
Carbon monoxide that produced by the total reaction in ATR need to be reduced their concentration by introducing water gas shift reaction and preferential oxidation reactions.

   a. Water gas shift
   Equilibrium reactors were placed to the plant to convert CO into carbon dioxide (CO_2). Three reactors were needed for conversion with water gas shift (WGS) reaction as the main reaction.

b. Preferential oxidation

To maximum reducing CO, preferential oxidation (PROX) reaction was introduced.

vi. Plant wide optimization

It was develop to optimized all the reactors used in the plant developed using Aspen HYSYS 3.2 and to reduced CO concentration to the specific requirement.

a. ATR optimization

It's used to optimize the ATR temperature outlet for heat integration.

b. Water gas shift optimization

It's used to optimize water molar flow to the ATR and reduces the CO concentration with WGS reaction.

c. Preferential oxidation optimization

It was formed to maintain the amount of air into PROX reactor that reduced the CO concentration to the specification.

vii. Temperature and component profile

The profile of temperature and components for every unit operations involve in this research was analyzed.

1.5 Thesis Organizations

This thesis involves the conclusion of the several tasks to achieve the objective. Chapter Two is discuss about the literature survey that related in synthesis of hydrogen for fuel cell applications. In this chapter, internal researched of hydrogen production using ethanol by autothermal reforming was been concentrated. This chapter is the major chapter because the development of the of hydrogen production are based on the literature survey that we had researched.

Chapter Three is about the methodology for the methods that we need in scope. Fundamentally, there are five methods that we carried out. The next chapter; Chapter Four, is optimization simulation of hydrogen production plant from ethanol for fuel cell application. We are using Aspen HYSYS 3.2 as a simulator to simulate the plant.

Chapter Five is the results and discussion based on the methodology that we use and developed from chapter four. Finally, Chapter Six is the conclusion all what we have done in this entire thesis.

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