SIMULATION AND OPTIMIZATION OF BUTANE AUTOTHERMAL REFORMER FOR FUEL CELL APPLICATIONS

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Dedicated to my family and friends

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ABSTRACT

Hydrogen (H_2) production has gaining popularity among researchers to aim a better future environment. H_2 is very excellent candidate to replace the existing fuel. Its high flammability and energy produced alongside no side product generated make it even more popular. The objective of the study is to develop a general steady-state simulation of H_2 production plant for fuel cell application using butane as the feedstock. The scopes of the study include stoichiometry mathematical calculations, base case steady-state simulation, base case simulation validation, a design of heat integration, carbon monoxide (CO) clean-up processes which contains water gas shift (WGS) and preferential oxidation (PrOx) reactors and plant wide optimization. The simulation has been run in Aspen HYSYS 2004.1 in steady-state mode in which optimization was done to generate more H_2 as well as CO reduction. The butane fuel processor was optimized at O/C ratio of 2.18 and S/C ratio of 4.6 to produce 39.2% of H_2 and has achieved 78.1% efficiency. While CO clean-up units was capable to reduce the CO concentration down to 10 ppm.

ABSTRAK

Penghasilan hidrogen (H_2) telah menjadi semakin popular dikalangan pengkaji-pengkaji bertujuan supaya alam sekitar menjadi lebih baik. H_2 adalah calon yang terbaik untuk menggantikan bahan bakar yang digunakan sekarang. Kebolebakarannya yang tinggi dan mengeluarkan tenaga yang banyak serta tidak menghasilkan produk sampingan menjadikan ia semakin popular. Objectif kajian ini ialah untuk membangunkan simulasi mod malar penghasilan H_2 melalui pengubah terhaba sendiri untuk aplikasi sel bahan bakar menggunakan butana sebagai bahan muatan. Skop-skop kajian ini termasuklah pengiraan matematik stoikiometri, simulasi keadaan-malar asas, pengesahan simulasi keadaan-malar asas, merekabentuk integrasi haba, proses pembersihan karbon monoksida yang mempunyai pertukaran gas berair (WGS) and pengoksidaan terpilih (PrOx) reaktor dan pengoptimuman loji keseluruhan. Simulasi telah dijalankan menggunakan perisian Aspen HYSYS 2004.1 dalam mod malar di mana pengoptimuman telah dilakukan supaya H_2 yang dihasilkan lebih banyak disamping mengurangkan CO. Pemproses bahan bakar butana ini berada pada keadaan optimum apabila nisbah O/C bernilai 2.18 dan nisbah S/C bernilai 4.6 yang mengandungi 39.2% H_2 yang mana kecekapannya telah mencapai 78.1%. Manakala unit-unit pembersihan CO telah dapat mengurangkan kepekatan CO sehingga 10 ppm.

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NOMENCLATURE

A = Heat transfer area

ATR = Autothermal reforming

a = Parameter, cubic equation of state

b = Parameter, cubic equation of state

Cp = Heat capacities, constant pressure

Cp^o = Standard heat capacities, constant pressure

F = Volumetric flow rate

g = Local acceleration of gravity

H = Molar or specific enthalpy $\equiv U + PV$

H^{ID} = Specific enthalpy of ideal gas

HTS = High temperature shift

ΔH = Enthalpy change (“heat”) of mixing; also, latent heat of phase transition

ΔH^o_{298} = Standard enthalpy change

i = Species

LTS = Low temperature shift

LHV = Lower heating value

MTS = Medium temperature shift

MW = Molecular weight

O/C = Oxygen-to-carbon ratio

P = Absolute pressure

P_o = Reference pressure

P_{ci} = Critical pressure, species i

P_{ri} = Reduced pressure, species i

$\bar{p}$ = Bias (steady-state) value

PrOx = Preferential oxidation

Q = Heat

$\dot{Q}$ = Rate of heat transfer

S = Molar or specific entropy

S^{ID} = Entropy of ideal gas

S/C = Steam-to-carbon ratio

T = Absolute temperature, Kelvins

T_n = Normal boiling point at 25°C, 1 atm

T_{ci} = Critical temperature, species i

T_{ref} = Reference temperature

T_{ri} = Reduced Temperature, species i

t = Time

U = Molar or Specific internal energy

V = Molar or specific volume

Z = Compressibility factor ≡ PV/RT

Superscript / Subscript

ID = Ideal gas

D = Derivative

i = Integral

av = Average

Greek letters

α = Function, cubic equation of state

μ = Viscosity

ρ = Density

ω = Acentric factor

η = Efficiency, %

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CHAPTER I

INTRODUCTION

1.1 Research Background

This study is mainly about general simulation of hydrogen (H_2) production for fuel cell application using butane as a raw material. The H_2 produced will be used in fuel-cell-powered vehicle that is known for its clean and recyclable fuel. In fact H_2 is the most abundant element that makes up over 90 percent of the matter of universe. When it is used as fuel, it will only produce water. It is such a good alternative to use H_2 as a fuel because of its colourless, odourless and extremely flammable gas and also the smallest and simplest member of the family of chemical elements compared with other fuel such as hydrocarbons, alcohols, or coals (Kothari et al., 2004).

Moreover, no side products are involved in the electrochemical conversions of H_2 with zero emission of hazardous species for instances volatile organic compound (VOCs), nitrogen oxides (NO_x) and carbon oxides (CO) (Darwish et al., 2004). The main goal of this study is to generate H_2 production on-board the vehicle from hydrocarbon feedstock. It is better than having H_2 in pressurized vessel or in cryogenic state for the reason that safety will be the major concern. Therefore, on-board conversion of butane into H_2 through an efficient and compact fuel processor is the main reason of this study.

1.2 Problem Statement

A simulation of butane reforming is scarce in the recent study for that reason a general simulation an optimization study of hydrogen production plant had been carried out. The aims of the study are to study preliminary design parameters for fuel cell processor, and investigate the H_2 production efficiency by using butane as a raw material and to clean carbon monoxide (CO) that produced prior to combustion and steam reforming reactions.

1.3 Objective and Scopes of the Study

The objective of this study is to develop a general steady-state simulation of H_2 production plant for fuel cell application using butane as the feedstock. In order to achieve the objective, scopes as shown below have been planned.

i. Stoichiometry mathematical calculation by using overall reaction to calculate inputs and outputs flow rate for fuel processor.

ii. Base case steady-state simulation was conducted in a selected simulator. In this scope, the data and reactions occurred in the autothermal reforming (ATR) reactor was set.

iii. Base case simulation validation was carried out. The purpose of this scope was to certify the overall reactions of ATR by distinguishing between calculated outputs composition and steady-state simulation outputs composition.

iv. Heat integration process was made to heat up the raw material to 100^{o}C before entering the ATR reactor. The design of heat integration could also minimize the heating requirement.

v. CO clean-up processes which contains water gas shift (WGS) and preferential oxidation (PrOx) reactors.

vi. Plant wide optimization where high H_2 generation as well as low CO concentration is needed for better hydrogen processor efficiency.

1.4 Thesis Organization

This thesis consists of 6 chapters. In Chapter 1, the introduction of the study is briefly discussed. While in Chapter 2 literature reviews from various sources are deeply understood to provide correct information prior to the simulation basis. Next is chapter 3 where the methodology of carrying the study is explained briefly. In addition to Chapter 3, Chapter 4 has more information about the study's requirements. Chapter 5 has the results and discussion of the simulation that indicate how the scopes of the study are achieved. To summarize this study, Chapter 6 was done to conclude the study and some recommendations were made.

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