ENVIRONMENT AND ECONOMIC ASSESSMENT OF HYDROGEN PRODUCTION FROM METHANE AND FROM ETHANOL

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SUPERVISOR’S DECLARATION

I hereby declare that I have checked this thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Master of Science

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STUDENT'S DECLARATION

I hereby declare that the work in this thesis is based on my original work except for quotations and citations, which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

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ABSTRAK

Permintaan bahan api fosil semakin meningkat dari tahun ke tahun tetapi sumber bahan api fosil berkurangan. Pada masa kini, para penyelidik cuba mencari sumber alternatif baru bagi mengurangkan kebergantungan terhadap bahan api fosil. Hidrogen merupakan salah satu bahan api alternatif yang menarik untuk dikaji. Tujuan kajian ini adalah untuk menilai terhadap kesan alam sekitar dan ekonomi bagi dua laluan proses penghasilan hidrogen iaitu metana (Kes1) dan etanol (Kes 2). Proses simulasi telah dijalankan dalam kajian ini dengan menggunakan perisian Aspen Plus versi 8.6. Reaksi stim reformasi metana dan etanol disimulasi berasaskan kepada tindakbalas kinetik. Data kinetik telah diperolehi melalui kajian literatur. Tindakbalas dilakukan dalam perisian Aspen Plus dengan menggunakan blok RPlug dengan menyusun kembali model kinetik Langmuir-Hinselwood-Watson (LHHW) dan model kinetic *power-law*. Pada masa yang sama, penulenan bagi hidrogen turut menggunakan kaedah simulasi. Pengesahsahihan data telah menunjukkan keputusan yang hampir sama dalam literatur. Selain itu juga, analisis sensitiviti juga telah dijalankan untuk melihat kesan beberapa parameter seperti suhu, tekanan, berat pemangkin dan nisbah masukan ke dalam rektor untuk kedua-dua kajian kes. Selepas itu, penilaian terhadap alam sekitar dan ekonomi telah dibuat. Data yang diperolehi telah digunakan untuk membuat perbandingan antara kedua-dua kajian kes. Penilaian kitaran hayat (LCA) telah digunakan dalam kajian ini untuk menilai kesan alam sekitar menggunak perisian GaBi menggunapakai kaedah ReCiPe untuk menilai impak alam sekitar bagi semua proses yang terlibat dalam kajian ini. Unit berfungsi bagi LCA dalam kajian ini adalah 1 kg untuk hidrogen. Secara keseluruhannya, 16 kategori impak telah dikaji dan hanya 3 menunjukkan kategori yang banyak memberi impak iaitu perubahan iklim, pengurangan fosil dan pengurangan air. Perbebasan gas rumah hijau tinggi untuk kes 2 iaitu 30.84 kg CO_2 eq. berbanding dengan kes 1 iaitu 9.44 kg CO_2 eq. Manakala, pengurangan fosil tinggi kes 2 iaitu 12.54 kg oil eq. berbanding kes 1 sebanyak 4.044 kg oil eq. Kes 2 juga menyebabkan penyusutan sumber air yang tinggi sebanyak 23.35 m^3 eq berbanding kes 1 sebanyak 4.01 m^3 eq. Penilaian ekonomi terhadap kedua-dua kajian kes telah dibuat. Kos modal untuk penghasilan hidrogen bagi kes 1 adalah kurang berbanding dengan kes 2 dengan perbezaan 7.92%. Manakala, kos utiliti untuk kes 1 lebih rendah berbanding kes 2 dengan perbezaan sebanyak 12.81%. Secara keseluruahannya, kes 1 iaitu hidrogen daripada metana adalah lebih mesra alam dan lebih jimat dalam kos CAPEX dan OPEX berbanding kes 2 walaupun daripada sumber tenaga yang boleh diperbaharui iaitu etanol.

ABSTRACT

The demand for fossil fuel increased year by year but the sources of fossil fuel is decreasing. Nowadays, researchers are looking at alternative energy sources to reduce the dependency on fossil fuel. Hydrogen is an interesting energy source alternative to be studied. The aim of this study is to perform environmental and economic assessment for two hydrogen production pathways namely from methane (Case 1) and ethanol (Case 2). Rigorous simulation of both processes was done using Aspen Plus version 8.6. The reaction of steam reforming from methane and ethanol were kinetic based simulation. The kinetic data was obtained from the literature. The reactions were modelled using RPlug blocks with rearranged Langmuir-Hinselwood-Hougen-Watson (LHHW) kinetic model and power law kinetic model. The purification of hydrogen was based on rigorous model in the simulation. The validation results show good agreement with results found in the literature. In addition, sensitivity analysis was carried out observing the effect of several parameters such as temperature, pressure, catalyst weight and feed ratio to the reactor performance for both cases. After that, environment and economic assessment were performed. The data obtained were used for comparison purposes. The environment assessment was based on life cycle assessment (LCA) to evaluate the environmental impact of all processes involved in hydrogen production using GaBi software based on ReCiPe method. The LCA functional unit used for both case studies was 1 kg of hydrogen. Overall, 16 categories impact assessment were carried out and only three were highly significant namely climate change, fossil depletion and water depletion. Case 2 shows high impact on climate change with 30.84 kg CO_2 eq compared to Case 1 with 9.44 kg CO_2 eq. On the other hand, Case 2 shows higher fossil fuel resource depletion with 12.54 kg oil eq compared to Case 1 with 4.044 kg oil eq. Furthermore, Case 2 also has a higher water resources depletion of 23.35 m^3 eq. compared to Case 1 which is only 4.01 m^3 eq. The capital cost for Case 1 is 7.92% less compared to Case 2. Meanwhile, the total utilities cost for Case 1 is 12.81% less compared to Case 2. In conclusion, the hydrogen production from methane, Case 1, is environmental friendlier and less costing in term of CAPEX and OPEX than Case 2..

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LIST OF SYMBOLS

A	Subscript
B	Subscript
C	Subscript
D	Subscript
Atm	Atmospheric pressure unit
˚C	Celsius
Cal/mol	Calories per mol
Bar	Pressure unit
g	Gram
kg	Kilogram
kw	kilowatt
kg/hr	Kilogram per hour
kmol/hr	Kilomole per hour
h	Hour
j	subscript
j/mol	Joule per mol
Ln	Natural logarithm
M	Subscript
m	meter
MJ/h	Megajoule per hour
m^2	Meter square
m^3	Meter cubic
MT/annum	Metric tonne per annum
MW	megawatt
CH_4	Methane
H_2O	Water
H_2	Hydrogen
CO	Carbon monoxide
CO_2	Carbon dioxide
MEA	Monoethanolamine
s	Seconds
$	US dollar

LIST OF ABBREVIATIONS

COMBRET	Combustion chamber
CAPEX	Capital Expenditure
CEPCI	Chemical Engineering plant cost index
C_P	Purchased cost
C_{TM}	Total module cost
C_{BM}	Base cost condition
C_{GR}	Grassroot cost
ESR	Ethanol steam reforming
Exp	Exponential
E-101	Heat exchanger 1 for Case 1
E-102	Heat exchanger 2 for Case 1
E-103	Heat exchanger 3 for Case 1
E-104	Heat exchanger 4 for Case 1
E-105	Heat exchanger 5 for Case 1
E-106	Heat exchanger 6 for Case 1
E-107	Reboiler stripper for Case 1
E-201	Heat exchanger 1 for Case 2
E-202	Heat exchanger 2 for Case 2
E-203	Heat exchanger 3 for Case 2
E-204	Heat exchanger 4 for Case 2
E-205	Heat exchanger 5 for Case 2
E-206	Heat exchanger 6 for Case 2
E-207	Reboiler stripper for Case 2
˚E	Enthalpy
ENTRL-RK	Electrolyte non-random two liquid model redhlich kwong
Eq.	Equivalent
FU	Functional unit
GHG	Greenhouse gas
GWP	Global warming potential
HWGS	High temperature water gas shift
LWGS	Low temperature water gas shift
k	Pre-exponential factor
k_1	Rate constant of MSR
k_2	Rate constant of WGS
K	Adsorption equilibrium
K_1	Adsorption equilibrium for CO
K_2	Adsorption equilibrium for H_2O
K_3	Adsorption equilibrium for CO_2
K_4	Adsorption equilibrium for H_2
LCA	Life cycle assessment
LHHW	Langmuir-Hinshelwood Hougen Watson
MSR	Methane steam reforming
N	Number of components
OPEX	Operating expenditure
P	Partial pressure
P_{CH4}	Partial pressure for CH_4
P_{H2O}	Partial pressure for H_2O

P_{H2}	Partial pressure for H_2
P_{CO}	Partial pressure for CO
P_{eth}	Partial pressure for ethanol
PFD	Process flow diagram
PSA	Pressure swing adsorption
R	Universal gas constant
R-101	Methane/Ethanol steam reforming reactor for Case 1
R-102	High temperature water gas shift reactor for Case 1
R-103	Low temperature water gas shift reactor for Case 1
R-201	Methane/Ethanol steam reforming reactor for Case 2
R-202	High temperature water gas shift reactor for Case 2
R-203	Low temperature water gas shift reactor for Case 2
RADFRAC	Rigorous distillation/separation column
RKSMHV2	RedhlichKwong Soave Modified huron Vidal mixing rule
SB1	System boundary 1
SB2	System boundary 2
SB3	System boundary 3
SB4	System boundary 4
SB5	System boundary 5
SB1-1	System boundary 1 for Case 1
SB1-2	System boundary 2 for Case 1
SB1-3	System boundary 3 for Case 1
SB1-4	System boundary 4 for Case 1
SB1-5	System boundary 5 for Case 1
SB2-1	System boundary 1 for Case 2
SB2-2	System boundary 2 for Case 2
SB2-3	System boundary 3 for Case 2
SB2-4	System boundary 4 for Case 2
SB2-5	System boundary 5 for Case 2
T	Absolute temperature
T_0	Reference temperature
T-101	Absorption column for Case 1
T-102	Stripper tower for Case 1
T-201	Absorption column for Case 2
T-202	Stripper tower for Case 2
WGS	Water gas shift
x_i	Mole fraction of component
y_i	Activity coefficient of component

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