COMPUTATIONAL APPROACHES FOR OPTIMAL DESIGN OF TAILOR MADE BIOFUEL BLENDS

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COMPUTATIONAL APPROACHES FOR OPTIMAL DESIGN OF TAILOR MADE BIOFUEL BLENDS

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Dedicated with deepest gratitude and heartfelt thanks
To my beloved family, for their endless love and care
To my angel Huppysha, for his infinite love and joy
To myself, for my hardwork and persistence
And to HIM for every second of my life.

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ABSTRACT

Diminishing fossil fuel supplies and increasing awareness on environmental issues surged the need for renewable and environmentally friendly alternative fuel options for the transportation sector. Diverse biofuel components can be produced from exploitation of biomass as an energy source. Malaysia having abundant palm biomass waste is prompted to efficiently utilize the available resources for production of second generation biofuel blends. However, complexity arises in designing suitable biofuel blends that comply to fuel regulation standards and generate reduced emissions while having equal performance as conventional diesel fuel. Experimental methods consume immense resources and time, require highly sophisticated equipments, and are difficult to conduct for fluid flow variations. Computational approaches adopt a systematic blend formulation process that assists on focused experimental work. In this study, optimal tailor made biofuel blends were designed and evaluated for engine performances, emissions, and in-cylinder fluid flow analyses through implementation of various computational approaches that follow an integrated framework. Systematic model based approach was applied to design tailor made biofuel blends that comply to EN590 fuel reference standard using B5 diesel, butanol, ethanol, and butyl levulinate as building blocks. Fuel blends were generated through Generalized Algebraic Modelling System and predicted fuel properties validated with experimental tests. In-cylinder fluid flow profiles were simulated through computational fluid dynamics model using ANSYS Fluent software version 13.0. Engine performances such as indicated power and indicated thermal efficiency were predicted through mathematical models where experimental validation was done for indicated power. Semi-empirical emission correlations were applied to predict nitrogen oxide, carbon monoxide, unburnt hydrocarbon, and smoke. Among the five tailor made biofuel blends formulated, Blend 4 was the most promising with enhanced performances and lower emissions in comparison to B5 diesel though nitrogen oxide emissions were higher.

ABSTRAK

Kemerosotan bekalan bahan api fosil dan peningkatan kesedaran terhadap isu-isu alam sekitar telah membangkitkan usaha berterusan untuk mencari bahan api alternatif yang mesra alam dan boleh diperbaharui bagi penggunaan di sektor pengangkutan. Pelbagai komponen bahan api bio dihasilkan daripada sisa buangan biojisim sebagai sumber tenaga. Malaysia antara negara pengeksport utama kelapa sawit kaya dengan sisa buangan kelapa sawit yang boleh digunakan secara cekap dan berkesan untuk penghasilan bahan api bio. Namun begitu, wujud kerumitan dalam merekabentuk bahan api bio yang mematuhi piawaian sekaligus menjana prestasi setanding diesel biasa dengan penghasilan emisi yang rendah. Kaedah eksperimen memakan masa dan sumber manakala variasi pembolehubah sukar dilaksanakan tanpa penggunaan peralatan canggih. Pendekatan komputasi pula mengikut proses berstruktur bagi pemilihan campuran bahan api bio dan ini membantu perjalanan eksperimen tertumpu. Kajian ini merekabentuk campuran optimum bahan api bio dan menilai prestasi enjin, penghasilan emisi serta menganalisis pengaliran bendalir di dalam enjin diesel melalui pelbagai jenis pendekatan komputasi yang mengikut satu rangka bersepadu. Pendekatan sistematik berasaskan model diaplikasi bagi merekabentuk campuran optimum bahan api bio yang mengandungi komponen-komponen B5 diesel, butanol, etanol, dan butil levulinat serta mematuhi piawaian EN590. Campuran optimum bahan api bio dijana menggunakan *Generalized Algebraic Modelling System* dan ciri-ciri khas yang diramal disahkan melalui kaedah eksperimen. Pengaliran bendalir di dalam enjin diesel disimulasi menggunakan program ANSYS Fluent versi 13.0. Prestasi enjin seperti kuasa dan kecekapan haba diramal menggunakan model matematik dan disahkan dengan keputusan eksperimen. Emisi nitrogen oksida, karbon monoksida, hidrokarbon tidak terbakar, dan asap pula diramal melalui korelasi empirikal. Antara lima campuran optimum bahan api bio yang dijana, Campuran 4 mempunyai prestasi enjin yang terbaik dan menghasilkan emisi rendah berbanding B5 diesel walaupun emisi nitrogen oksidanya agak tinggi.

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LIST OF SYMBOLS

A	-	Area of piston head
Actual	-	Tailor made biofuel blend property from experiment
$BLlimit_j$	-	Composition of butyl levulinate in fuel blend mixture j
calf	-	Objective function to maximize calorific value of fuel blend
C_i	-	Raw material cost of fuel blend component i
CN_i	-	Cetane number of fuel blend component i
CN_j	-	Cetane number of fuel blend mixture j
cst	-	Objective function to minimize total fuel blend cost
CV	-	Fuel calorific value
CV_i	-	Calorific value of fuel blend component i
CV_j	-	Calorific value of fuel blend mixture j
$density_j$	-	Density of fuel blend mixture j
d_b	-	Cylinder bore diameter
DT_i	-	Distillation temperature of fuel blend component i
DT_j	-	Distillation temperature of fuel blend mixture j
$ethanollimit_j$	-	Composition of ethanol in fuel blend mixture j
f_{max}	-	Maximizing function
f_{min}	-	Minimizing function
I	-	Turbulence intensity
ip	-	Indicated power
K	-	Number of cylinders
k	-	Turbulence kinetic energy
L	-	Length of stroke
L_T	-	Total length of combustion chamber
$\dot{m}_f$	-	Fuel mass flow rate
N	-	Engine speed

n	-	Number of power strokes per minute
η_{ith}	-	Indicated thermal efficiency
O_2 *content*	-	Amount of fuel-bound oxygen
ρ	-	Fuel density
ρ_i	-	Density of fuel blend component *i*
p_{im}	-	Indicated mean effective pressure
Predicted	-	Tailor made biofuel blend property from GAMS
r	-	Compression ratio
S_i	-	Sulphur content of fuel blend component *i*
S_j	-	Sulphur content of fuel blend mixture *j*
μ	-	Kinematic viscosity of fuel
μ_i	-	Kinematic viscosity of fuel blend component *i*
u_{avg}	-	Mean flow velocity
υ_i	-	Volume fraction of fuel blend component *i*
$viscosity_j$	-	Kinematic viscosity of fuel blend mixture *j*
V_c	-	Combustion chamber clearance volume
V_s	-	Displacement volume
V_T	-	Total cylinder volume
z_j	-	Total cost of fuel blend mixture *j*

Greek Letters

$\sum$	-	Summation

Subscripts

i	-	Index for pure fuel blend components
j	-	Index for tailor made biofuel blend mixture

LIST OF ABBREVIATIONS

ABE	-	Acetone-Butanol-Ethanol
ANN	-	Artificial Neural Networks
AP/OA/ER	-	Augmented Penalty-Outer Approximation-Equality Relaxation
APE	-	Absolute Percentage Error
ASF	-	Advanced Sizing Functions
ASTM	-	American Society for Testing and Materials
BARON	-	Branch-And-Reduce Optimization Navigator
BDC	-	Bottom Dead Centre
BL	-	Butyl Levulinate
CFD	-	Computational Fluid Dynamics
CI	-	Compression Ignition
CN	-	Cetane Number
CO	-	Carbon Monoxide
CO_2	-	Carbon Dioxide
DBS	-	Density Based Solver
DI	-	Direct Injection
EN	-	European Standard
FAME	-	Fatty Acid Methyl Ester
GAMS	-	Generalized Algebraic Modelling System
GINO	-	General Interactive Optimizer
HC	-	Unburnt Hydrocarbon
IC	-	Internal Combustion
IDI	-	Indirect Injection
MATLAB	-	Matrix Laboratory
MIXD	-	Mixture Design Routine
NLP	-	Non-Linear Programming

NO	-	Nitrogen Oxide
NO_x	-	Oxides of Nitrogen
OQ	-	Orthogonal Quality
PBS	-	Pressure Based Solver
PCA	-	Principal Component Analysis
PCR	-	Principal Component Regression
POME	-	Oil Palm Mill Effluent
PPD	-	Product-Process Design
rpm	-	Revolutions per Minute
SI	-	Spark Ignition
SIMPLE	-	Semi-Implicit Method for Pressure-Linked Equations
SO_2	-	Sulphur Dioxide
TDC	-	Top Dead Centre

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

Since decades, conventional fossil fuels such as petroleum, natural gas, and coal have played important roles in satisfying the ever increasing world energy demands. Transportation sector alone consumes nearly one third of global energy supplies. However, supply of conventional fossil fuels is finite and are fast depleting. On top of that, increased awareness on environmental issues have caused an outburst of search for alternative vehicular fuel options which are environmentally friendly, renewable, and sustainable. Biofuel has pioneered the alternative fuel sector for some time now owing to studies conducted on tapping potential of biomass as a primary energy source. Biofuels produced from biomass are categorized under second-generation biofuels which evade the fuel versus food controversy.

Amid neighbouring countries such as Thailand, Philippines, and Indonesia promoting the use of second-generation biofuels, Malaysian government introduced its fifth fuel strategy under the Eighth Malaysian Plan (Malaysia, 2001). The fifth fuel strategy promoted use of renewable energy with focus on biomass as an energy source. Malaysia further enhanced her initiatives towards developing renewable energy from biomass resources with implementation of National Biofuel Policy in2006 under the Ninth Malaysian Plan (Malaysia, 2006). The latest instalment was the introduction of National Biomass Strategy 2020 which focuses on fully utilizing all types of biomass feedstock available in the country with emphasis on oil palm biomass. A mandate for blend of five percent palm methyl ester in diesel, commonly known as B5 diesel, was introduced in 2011 parallel to the policy.

Malaysia is the world's second largest producers of palm oil which generates surplus palm biomass waste (Naik *et al.*, 2010; Ng *et al*., 2012). Biomass is generally composed of lipid and cellulosic materials. Various conversion routes can be used to process biofuels using these components as starting materials. Bioalcohols, biodiesel, bio-oils, bio-ethers, bio-esters, and synthetic hydrocarbons make up basic building blocks for liquid biofuels. Among these, biodiesel and bioalcohols are widely commercialized with bio-esters appearing as attractive new biofuel blend option.

However, vast and infinite possibilities of biofuel blend candidates cause complexity in design. Implementation of biofuel blends as vehicular fuel requires the fuel to meet necessary criteria which will facilitate existing engines to operate on the new fuel blends with little or no modification. Composition of fuel blends gravely influence fuel properties that play significant role in combustion activities, engine performance and exhaust emissions. Experimental methods evaluating competency of biofuel blends consume immense time and resources. Computational approaches adopting a structured candidates selection process saves time and resources through focused experimental work.

Mathematical models, empirical correlations, phenomenological models, computational fluid dynamic models, and black-box approaches have been widely used in numerous studies that assess biofuel blends. In this study, combination of several computational approaches were implemented to design and evaluate tailor made biofuel blends that fulfil criteria for use as vehicular fuel in diesel engine.

1.2 Problem Statement

Designing novel biofuel blends is a complex process credits to the infinite possibilities of biofuel blend components. It is a necessity that the tailor made biofuel blend properties conform to fuel regulation standards in order to be functional as vehicular fuel in standard diesel engines. Experimental methods are performed through trial-and-error which is tedious and time consuming due to the wide range of potential biofuel blend candidates. It is also cost ineffective as it consumes huge amount of resources in the course of ensuring fuel properties are in compliance with fuel regulation standards. Therefore, a systematic methodology model-based approach was implemented to minimize the candidates search region and generate tailor made biofuel blends. Resources and time can be saved through focused experimental work.

In-cylinder fluid flow characteristics are very much influenced by fuel properties. It has also been established to control engine performances and exhaust emissions. However, fluid flow in a diesel engine combustion chamber is a challenging area of study due to numerous factors that cause flow variations. Experimental methods are focused on particular parts of the chamber such as at the fuel injector with emphasis being on fuel spray characteristics and valve lift. Mathematical models follow similar approach. Black-box approaches are more versatile but in-cylinder fluid flow profiles cannot be clearly analyzed. Therefore, computational fluid dynamics (CFD) were introduced in this study to model and simulate in-cylinder fluid flow profiles that are affected by fuel blend properties as CFD models can be implemented when fine flow details are not required. In-addition, CFD software is equipped with phenomenological models that are adequate to predict fluid flow motions.

Engine performances and exhaust emissions of tailor made biofuel blends are necessary parameters for competency evaluation. Assessment through experimental tests are again costly and consume resources and time. Furthermore, highly sophisticated test equipments are required for analysis of certain exhaust emissions such as sulphur oxides and particulate matters which may render it unavailable at most engine test beds. Hence in this study, mathematical models based on thermodynamic analysis of an engine cycle was implemented to predict engine performance parameters. Emissions were predicted through semi-empirical correlations designed in a study by Ng *et al*. (2012) with a 85% success rate for tailor made biofuel blends with particular ranges of fuel properties.

Generally, design of novel biofuel blends are segregated and focused on one particular area of interest. Studies will either be conducted on fuel blend properties such as those by Benjumea *et al*. (2008), Jenkins *et al*. (2013), and Al-Hamamre and Al-Salaymeh (2014) or on engine performance and exhaust emissions like those by Yusaf *et al*. (2011), Giakoumis *et al*. (2013), and Atmanli *et al*. (2014) to name a few. On the other hand, studies on in-cylinder fluid flow profiles are totally independent with findings relating only to fuel properties, for instance studies by Battistoni and Grimaldi (2012) and Mohan *et al*. (2014). Therefore, this study introduces an integrated methodology that combines the fore mentioned computational approaches to design tailor made biofuel blends and evaluate engine performances, emissions, and in-cylinder fluid flow profiles for use as vehicular fuel option.

1.3 Objectives of Study

The main objective of this study is to design optimal tailor made biofuel blends as alternative vehicular fuel options for diesel engines in Malaysia. The sub-objectives include:

(i) Development of an integrated framework for biofuel blending design.

(ii) Evaluation of performance and emissions of the designed tailor made biofuel blends.

(iii) Analysis of in-cylinder fluid flow motion of the designed tailor made biofuel blends.

1.4 Scopes of Study

In order to achieve objectives of this study, scopes of study were identified as the following:

(i) Identifying and selecting physical properties of biofuel blends that significantly affect in-cylinder fluid flow motion, engine performances, and exhaust emissions of a diesel engine. Density, kinematic viscosity, cetane number, calorific value, and distillation temperature were selected.

(ii) Generating tailor made biofuel blends through a systematic methodology model-based approach using Generalized Algebraic Modelling System (GAMS). Tailor made biofuel blends were generated to comply with EN590 fuel reference standard. Generated fuel blend properties were validated with experimental tests conducted according to the American Society for Testing and Materials (ASTM) standard.

(iii) Analyzing effects of fuel blend properties towards in-cylinder fluid flow motion through computational fluid dynamics. YANMAR TF120M diesel engine combustion chamber was modelled and fluid flow motion simulated through implementation of ANSYS Fluent software.

(iv) Predicting engine performance for tailor made biofuel blends using mathematical models and comparing with B5 diesel. Engine performance parameters predicted were indicated power which was validated with experimental results and indicated thermal efficiency.

(v) Predicting exhaust emissions for tailor made biofuel blends using semi-empirical correlations designed and implemented in a study by Ng *et al*. (2012). Emissions predicted include nitrogen oxide, carbon monoxide, unburnt hydrocarbon, and smoke opacity.

1.5 Contribution of Study

Key contribution of this study is a new integrated framework applicable for designing tailor made biofuel blends functioning as alternative fuel for diesel engine vehicles in Malaysia. Experimental validation of predicted fuel properties, effects of fuel properties towards in-cylinder fluid flow motion, and evaluation of performance and emissions enable this study to be notable from previous studies that implement existing product design frameworks. Hence, this study is expected to contribute greatly towards future work on designing optimal tailor made biofuel blends for commercial use. Appendix A highlights all publications related to contribution of this study.

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