GREEN DIESEL BLENDS DESIGN USING DECOMPOSITION-BASED OPTIMIZATION APPROACH

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Specially dedicated to my parents, family and friends

Thanks for their support and encouragement along the journey

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ABSTRACT

Petrodiesel-biofuel/biochemical blend (green diesel blend) is a promising solution in reducing environmental impact while improving the performance of petrodiesel. A systematic computer-aided approach can efficiently solve green diesel blends' design problems to replace the iterative, costly and time-consuming experimental trial-and-error approach. Other than the engine performance related fuel properties (density, kinematic viscosity, cetane number and higher heating value), the safety indicator: flash point is an important safety consideration for diesel fuel and it should be considered in the green diesel blend design to avoid fire accident. The aims of this study are to develop a systematic computer-aided tailor-made green diesel blend design algorithm and to improve the flash point prediction model, which is the Liaw model for B5 palm oil biodiesel (B5)-ester/ether/alcohol blends. The algorithm contains two main phases: the model-based design and the experimental validation. The optimum green diesel blend is computationally optimized in the model-based design phase. The accuracy of the Liaw model using UNIFAC type models is improved for B5-ester/ether/alcohol by regressing the UNIFAC group interaction parameters. The verified and improved Liaw models are embedded into the model-based design phase to optimize the green diesel blend. The physicochemical property, engine performance and emissions of the optimum blend obtained in the model-based design phase are experimentally validated in the experimental validation phase. The application of the developed design algorithm is illustrated by finding the right combination of the binary and ternary blends of B5-ester/ether/alcohol. The ideal Liaw model, the Liaw model using the original UNIFAC and the Liaw model using original UNIFAC with parameters set B (group interaction parameter between CH_2 and OH are revised) are used to predict the flash points of the B5-ether, B5-ester and B5-alcohol blends. GB3 (B5-11.1 % by mass of diethyl succinate) and GT1 (B5-24.1% octanol-5.9 % diethyl succinate, by mass %) with or without the cetane enhancer: 2-ethylhexyl nitrate (2EHN) are the optimum binary and ternary blends with the high oxygen content obtained in the model-based design phase. Satisfactory experimental validation results were obtained in experimental validation phase and GT1A (GT1-0.17 % by mass of 2EHN)) was identified to be the most promising green diesel blend owning to its lower emissions of nitrogen oxide (19.21 % lower than B5), un-burnt hydrocarbon (27.48 % lower than B5) and carbon monoxide (36.73 % lower than B5). Meanwhile, GT1A has comparative fuel efficiency to B5. The developed green diesel blend design algorithm serves as an improved model for solving green diesel blend design problem.

ABSTRAK

Adunan petrodiesel-bahan api bio/biokimia (adunan diesel hijau) ialah penyelesaian yang menjanjikan pengurangan impak terhadap alam sekitar serta meningkatkan prestasi petrodiesel. Pendekatan berbantukan komputer yang bersistematik dapat menyelesaikan secara cekap masalah reka bentuk adunan diesel hijau untuk menggantikan kaedah cuba dan jaya secara eksperimen yang melibatkan lelaran, mahal dan mengambil masa. Selain daripada prestasi enjin yang berkaitan dengan sifat-sifat bahan api (ketumpatan, kelikatan kinematik, nombor setana dan nilai pemanasan tinggi), penunjuk keselamatan: takat kilat ialah satu pertimbangan keselamatan yang penting bagi bahan api diesel dan ia perlu dipertimbangkan di dalam reka bentuk adunan diesel hijau untuk mengelakkan kemalangan kebakaran. Kajian ini bertujuan untuk membangunkan satu algoritma reka bentuk adunan diesel hijau buatan-sesuaian berbantukan komputer yang bersistematik dan memperbaiki model ramalan takat kilat, iaitu model Liaw bagi adunan biodiesel minyak sawit B5 (B5)-ester/eter/alkohol. Algoritma tersebut mengandungi dua fasa utama: reka bentuk berasaskan model dan pengesahan eksperimen. Adunan diesel optimum hijau dikirakan secara berkomputer dalam fasa reka bentuk berasaskan model. Ketepatan model Liaw yang menggunakan model jenis UNIFAC dipertingkatkan melalui regresi parameter interaksi kumpulan UNIFAC bagi B5-ester/eter/alkohol. Model Liaw yang telah disahkan dan diperbaiki kemudiannya dibenamkan ke dalam fasa reka bentuk berasaskan model untuk mengoptimumkan adunan diesel hijau. Sifat fizikokimia, prestasi dan pelepasan enjin bagi adunan optimum yang diperoleh pada fasa reka bentuk berasaskan model disahkan secara eksperimen dalam fasa pengesahan eksperimen. Penggunaan algoritma reka bentuk yang telah dibangunkan ini ditunjukkan dengan mencari kombinasi yang betul bagi adunan perduaan dan pertigaan B5-ester/eter/alkohol. Model Liaw unggul, model Liaw yang menggunakan UNIFAC asal dan model Liaw yang menggunakan UNIFAC asal dengan parameter set B (parameter interaksi antara kumpulan CH_2 dan OH yang telah disemak semula) digunakan untuk meramalkan takat kilat bagi adunan B5-eter, B5-ester dan B5-alkohol. GB3 (B5-11.1 % jisim dietil suksinat) dan GT1 (B5-24.1 % jisim oktanol-5.9 % jisim dietil suksinat) dengan atau tanpa penggalak setana: 2-etilheksil nitrat (2EHN) ialah adunan perduaan and pertigaan optimum dengan kandungan oksigen yang tinggi yang diperoleh di fasa reka bentuk berasaskan model. Keputusan pengesahan eksperimen yang baik telah diperoleh pada fasa pengesahan eksperimen dan GT1A (GT1-0.17% jisim 2EHN)) dikenalpasti sebagai adunan diesel hijau yang terbaik kerana ia dapat mengurangkan pelepasan nitrogen oksida (19.21 % lebih rendah daripada B5), hidrokarbon tidak terbakar (27.48 % lebih rendah daripada B5) dan karbon monoksida (36.73 % lebih rendah daripada B5). Sementara itu, GT1A mempunyai prestasi enjin yang setanding dengan B5. Algoritma reka bentuk adunan diesel hijau yang telah dibangunkan menyediakan satu model diperbaiki untuk menyelesaikan masalah reka bentuk adunan diesel hijau.

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LIST OF ABBREVIATIONS

AAD	-	average absolute deviation
AARD	-	average absolute relative deviation
ASTM	-	American Society of Testing and Materials
BL	-	butyl levulinate
BMEP	-	brake mean effective pressure
BSFC	-	brake specific fuel consumption
BTE	-	brake thermal efficiency
BU	-	1-butanol
BUDIOL	-	1,4-butanediol
B5	-	B5 palm oil biodiesel
CAMD	-	computer-aided molecular design
C=C	-	bonded alkyl chains
CCOO	-	esters group
CEN	-	European Committee for Standardization
CH_2	-	alkyl chains
CN	-	cetane number
CO	-	carbon monoxide
CO_2	-	carbon dioxide
DBE	-	dibutyl ether
DES	-	diethyl succinate
DGDE	-	diethylene glycol diethyl ether
DME	-	dimethyl ether
DPE	-	dipentyl ether
DTBP	-	di (tert-butyl) peroxide
EGR	-	exhaust gas recirculation
2EHN	-	2-ethylhexyl nitrate
EL	-	ethyl levulinate

EPA	-	Environmental Protection Agency
Eq.	-	equation
Exp.	-	experimental values
FAME	-	fatty acid methyl esters
F.B	-	free bound
FP	-	flash point
FT	-	Fischer-Tropsch
GAMS	-	Generalized Algebraic Modeling System
GHG	-	green house gases
HE	-	1-hexanol
HHV	-	higher heating value
LLE	-	liquid-liquid equilibrium
LPG	-	Liquefied Petroleum Gas
M	-	miscible
MATLAB	-	Matrix Laboratory
MINLP	-	Mixed Integer Non-linear Programming
N_2	-	nitrogen
NO	-	nitrogen monoxide
NO_x	-	nitrogen oxides
N_2O	-	nitrous oxide
NO_2	-	nitrogen dioxide
N_2O_2	-	di-nitrogen dioxide
N_2O_3	-	di-nitrogen trioxide
N_2O_4	-	di-nitrogen tetroxide
N_2O_5	-	di-nitrogen pentoxide
NRTL	-	non- random two-liquid
OCT	-	1-octanol
OH	-	alcohol group
P	-	partial miscible
PEN	-	1-pentanol
PENDIOL	-	1,5-pentanediol
PM	-	particulate matter
POM	-	palm oil biodiesel

PV	-	pentyl valerate
ppm	-	part per million
Prep.	-	prediction values
QSPR	-	quantitative structure-property relationships
RSM	-	response surface methodology
rpm	-	revolution per minute (indicate engine speed)
SO_x	-	sulfur oxides
SO_2	-	sulfur dioxides
SO_3	-	sulphur trioxide
T_b	-	boiling point
T_m	-	melting point
UHC	-	un-burnt hydrocarbon
ULSD	-	ultra-low sulfur diesel
UNIFAC	-	universal functional activity coefficient
UNIQUAC	-	universal quasichemical
VLE	-	vapor liquid equilibrium

LIST OF SYMBOLS

A, B, C	-	parameter of Antoine equation
$AARD$	-	average absolute relative deviation
$a_{m,k}$, $b_{m,k}$, $c_{m,k}$	-	group interaction parameter of UNIFAC type models
$BSFC$	-	brake specific fuel consumption
BTE	-	brake thermal efficiency
Brake Power	-	brake Power
c	-	intercept of tangent plane
CN	-	cetane number
$engine\ speed$	-	engine speed
F_{obj}	-	objective function
$fuel\ consumption$	-	fuel consumption
ΔG_{mix}	-	Gibbs energy of mixing
HHV	-	higher heating value
H_2O	-	water content
heat input by fuel	-	heat input by fuel
m , *k*	-	main group for UNIFAC type models
max	-	maximize
min	-	minimize
N	-	total number of experimental data points
n	-	number of components
OC	-	oxygen content
P^{sat}	-	saturated vapor pressure
$P_{i,FP}^{sat}$	-	vapor pressure of substance *i* at its flash point
T	-	temperature
T_{FP}	-	flash point

$T90$	-	distillation temperature at 90 volume % of distillate recovered
$T95$	-	distillation temperature at 95 volume % of distillate recovered
$Torque$	-	torque
TPD	-	tangent plane distance
t	-	slope of tangent plane
x	-	mass fraction
x_{Fbio}	-	the final maximum feasible composition of blending agent
x_{Lbio}	-	maximum blending agent composition that match the linear property constraints
x_{NLbio}	-	maximum blending agent composition that match the non linear property constraints
x_{Pbio}	-	maximum blending agent composition that is miscible with B5
xm	-	mole fraction
η	-	kinematic viscosity
ρ	-	density at 15 °C
ζ	-	target properties
γ	-	activity coefficient
$\sum$	-	summation
$\forall$	-	entire
>	-	greater than
>>	-	much more greater than

Subscripts

B5	-	B5 palm oil biodiesel
BU	-	1-butanol
bio	-	Biofuel/bio-chemical (blending agent)
com	-	components
D	-	petrodiesel
DBE	-	dibutyl ether

DGDE	-	diethylene glycol
DPE	-	dipentyl ether
EL	-	ethyl levulinate
e	-	compound *e*
exp	-	experimental value
FP	-	flash point
f	-	compound *f*
GB	-	green diesel
HE	-	1-hexanol
i	-	compound *i*
mix	-	mixture
LLE	-	liquid-liquid equilibrium
PEN	-	1-pentanol
POM	-	palm oil biodiesel
$pred$	-	predicted value
VLE	-	vapor-liquid equilibrium

Superscript

α, β	-	two coexist phase at liquid-liquid equilibrium

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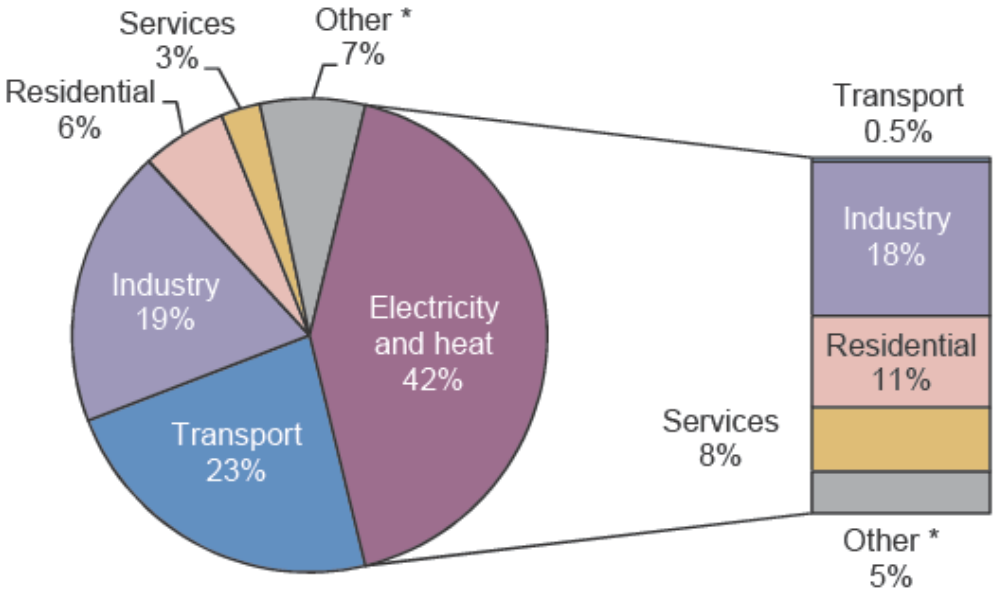
CHAPTER 1

INTRODUCTION

1.1 Research Background

Fossil fuel remains the main energy resource for transportation (majorly gasoline and petrodiesel) (IPCC, 2007); however, it is the largest source of the main green house gases (GHG) emissions: carbon dioxide (CO_2) after coal (IEA, 2015). In year 2013, the transportation sector alone was responsible for around 23 % of world CO_2 emissions (see Figure 1.1) and road transport was the major CO_2 contributor compared to the other transportations (see Figure 1.2) (IEA, 2015). CO_2 emission is unlikely to reduce in the foreseeable future as the demand of the transportation fuel is projected to grow up to nearly 40 % in year 2035, with the increasing population (IEA, 2013).

Other than CO_2 emissions, other emissions such as particulate matter (PM), nitrogen oxides (NO_x), carbon monoxide (CO), un-burnt hydrocarbon (UHC) and sulfur oxide (SO_x) have posed concerns. The main cause and the side-effects of these emissions to environment and human are listed in Table 1.1. Diesel vehicle have lower CO and UHC than petrol vehicle; however, diesel vehicle has much higher PM, NO_x and SO_x when compared to petrol vehicle (Lee *et al.*, 2011). These emissions are carcinogens, especially for the respiratory suspended PM. Consequently, World Health Organization recognizes these diesel vehicle emissions as carcinogen, and these emissions are identified as the source of atmospheric haze (Geng *et al.*, 2014).



*include fishing, energy industries other than heat generation and electricity, forestry or agriculture and other not specified emissions

Figure 1.1: World CO_2 emissions (IEA, 2015)

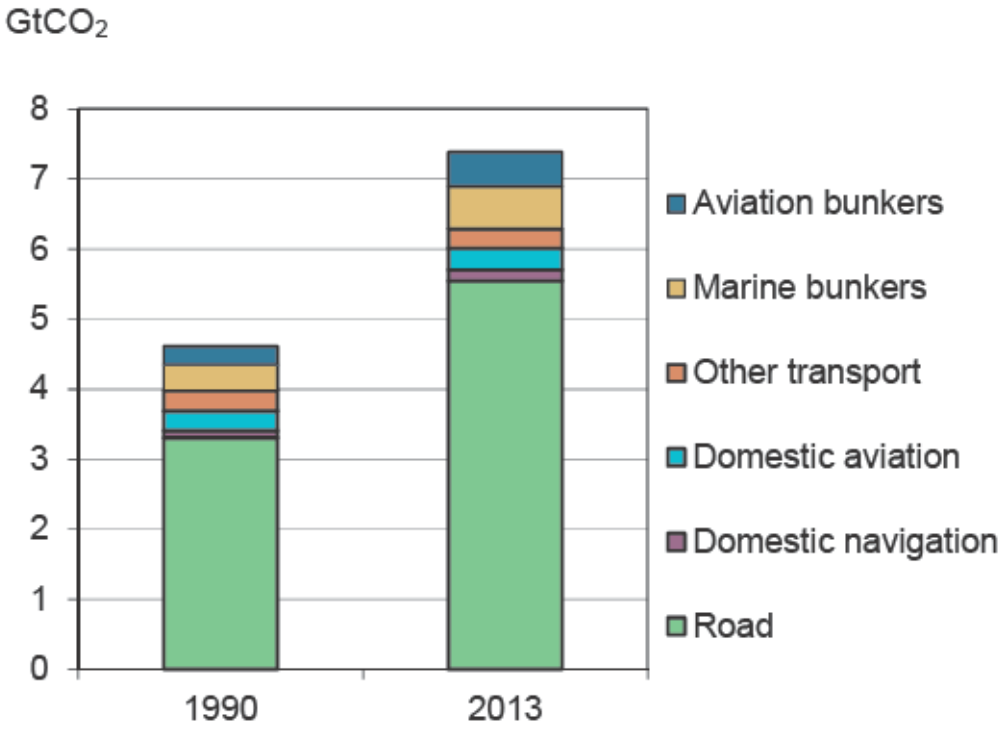


Figure 1.2: CO_2 from different transportation (IEA, 2015)

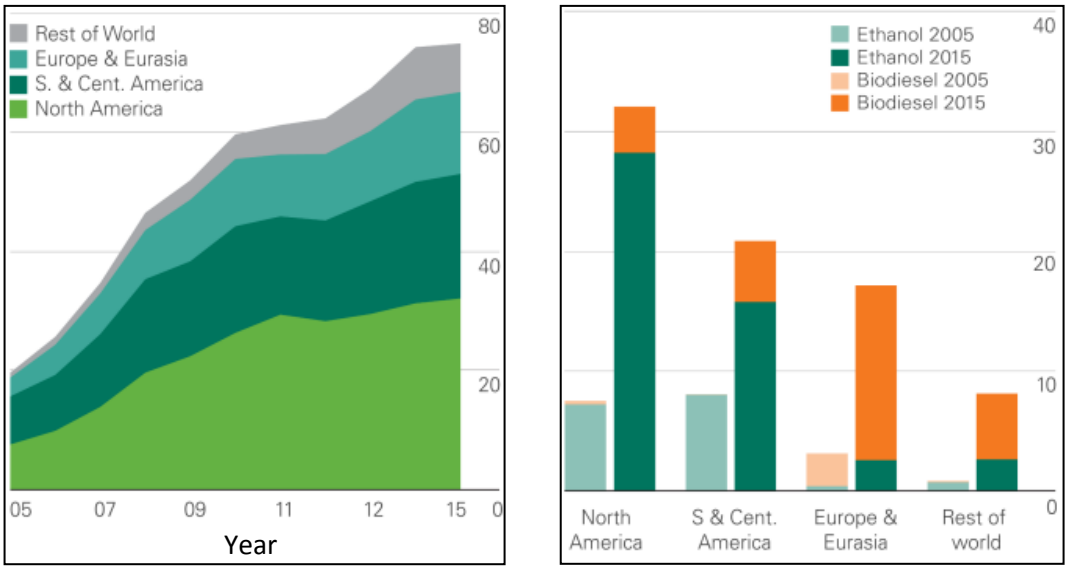
Table 1.1: The main pollutants from diesel fuel

Pollutant	**Formation**	**Side-Effect**
Particulate matter, PM	result of incomplete combustion (Kim *et al.*, 2002)	severe effect to environment and human health as it could lead to asthma, lung cancer and increased blood pressure (Geng *et al.*, 2014)
Nitrogen oxide, NO_x	formed when diesel combusts in high temperature (Sayin, 2010)	leads to respiratory problem and it causes the formation of PM, acid rain, smog and ground level ozone, which are adversely affecting human health (Icopal, 2016)
Carbon monoxide, CO	is a product of incomplete burning of fuel due to insufficient air supply (Sayin, 2010)	has the potential to form ground level ozone and can cause neurological damage and harm to unborn baby if expose to low CO concentration for a long term (SEPA, 2016)
Un-burnt hydrocarbon, UHC	formed when the un-burned or partially burned fuel is released from diesel engine	toxic and carcinogenic; it can react with NO_x under sunlight to form ozone (MED, 2016)
Sulphur oxide, SO_x	generated because of the combustion of the sulfur-containing compounds, which is naturally present in petrodiesel fuel.	is the precursor of acid rain and it affects respiratory system (Queensland Government, 2016)

In order to mitigate these carcinogenic diesel emissions (see Table 1.1), a greener alternative energy resource is essential. Biofuel is one of the promising solutions to address this emission issue. Biofuel is renewable; it can be derived from any biomass including vegetable oil, agriculture waste (e.g. rice straw and empty fruit branch) and any lignocellulosic resources. Using biofuel to run diesel vehicle prompts to CO_2 equivalence as the CO_2 generated by a running diesel vehicle can be offset by plant for photosynthesis (Tan *et al.*, 2011). On the other hand, nearly zero sulfur containing compounds are present in biofuel; hence, the issue regarding SO_x emissions is mitigated (Yaakob *et al.*, 2013). The oxygen bonded biofuel provides lean-combustion by its self-provided oxygen; therefore, it can potentially reduce the emissions of PM (Zhang *et al.*, 2016), CO (Li *et al.*, 2014) and UHC (Atmanli *et al.*,

2015). In addition, most biofuel could lower the combustion temperature and NO_x emission can be reduced (Chang *et al.*, 2013).

The world of biofuel production has grown positively since 2005 as illustrated in Figure 1.3. Biodiesel is the main biomass renewable fuel produce for petrodiesel replacement as compared to other biofuel such as alcohol. Biodiesel is majorly produced by transesterification of vegetable oil with alcohol, mainly methanol (Aransiola *et al.*, 2014). The world biodiesel production is still mainly relying to the edible oil and this biodiesel is recognized as the first generation biofuel as it is from edible resources (Larson, 2008, Demirbas, 2009). Malaysia is one of the representatives from the Asian countries to produce biodiesel using palm oil. Nowadays, the second generation biofuel, which is produced from non-edible resources and waste biomass (lignocellulosic material), has become more important. Thermochemical (pyrolysis, gasification) and biochemical (fermentation) processes are the common production routines to convert the lignocellulosic material into valuable biofuel (Schlichter and Montes, 2011), for example alcohols (e.g. bioethanol, biomethanol, biobutanol and linear bioalcohol mixed), Fischer-Tropsch renewable diesel (a mixture of carbon chains), ethyl levulinate (Huber *et al.*, 2006), dimethyl ether (Chen *et al.*, 2012) etc.



(a) global biofuel production by region in million tonnes oil equivalent

(b) global biofuel production by types in million tonnes oil equivalent

Figure 1.3: Global biofuel production (BP, 2016)

Biofuel could efficiently reduce harmful emissions, but being able to fully replace petrodiesel with biofuel is undesired. Biodiesel have higher viscosity than petrodiesel fuel; it will cause engine filters clogging and engine modification is needed to run diesel engine with biodiesel (Sorate and Bhale, 2015). Dimethyl ether has totally different physical properties with petrodiesel hence the storage and fuel transport and injection system are needed to alter (Kim *et al.*, 2011, Semelsberger *et al.*, 2006). Furthermore, green diesel (Kordulis *et al.*, 2016) and Fischer-Tropsch renewable diesel (Im-orb *et al.*, 2016) have similar physicochemical properties with diesel; however, new refinery plant is required for large scale production. These vast technology evolutions lead to unaffordable implementation cost and immediately stopping the petrodiesel supply that is not economically feasible. Hence, blending petrodiesel with biofuel or bio-chemical becomes beneficial.

Tailor-made green diesel blend, which is interpreted as the blend of petrodiesel with oxygenated biofuel/bio-chemical (bio-ester, bio-ether and bio-alcohol), is superior to reduce harmful emission while retaining or even improving the engine performance with acceptable implementation cost. Biofuel/bio-chemical acts as the oxygenate 'additive' to petrodiesel to enhance complete fuel combustion; hence, reduces the most carcinogenic emissions like PM, UHC and CO in the exhaustion stream. For instance, biodiesel-petrodiesel blend is a commercial tailor-made green diesel blend. This blend has been commercialized in European Union, United States and Asian countries including Malaysia. Biodiesel-petrodiesel blend does not only reduce harmful diesel emissions; it prolongs engine life by improving the lubricity of petrodiesel fuel (Knothe and Steidley, 2005). Unfortunately, biodiesel-petrodiesel blends generally have higher NO_x than petrodiesel (Can *et al.*, 2016). Furthermore, enhancing the combustion and fuel properties of this green diesel blend to attain greener and more efficient fuel is important.

Nowadays, green diesel blends containing lignocellulosic biofuel/bio-chemicals, such as bio-ester, bio-ether and bio-alcohol are getting more attention due to their excellent fuel properties (Koivisto *et al.*, 2015), (Chauhan *et al.*, 2016) and (Campos-Fernández *et al.*, 2012a). In addition, utilization of lignocellulosic biofuel/bio-chemical mitigates the conflict between food and fuel as the current

biodiesel production is mainly relying on edible vegetable oil. Blending oxygenated biofuel/bio-chemicals with petrodiesel can significantly reduce harmful emissions; however, it might deteriorate the fuel combustion quality by reducing both cetane number (CN) and higher heating value (HHV) of petrodiesel. This happened because biofuel/bio-chemical generally has lower HHV and CN than petrodiesel. Using diesel fuel with lower HHV and CN will leads to higher fuel consumption (Pandey *et al.*, 2012) and engine knocking (Lim *et al.*, 2012). In order to reduce the harmful emissions without significantly drop the fuel quality, the main concerns always related to tailor-made green diesel blend design problem are on how to define the blend target properties and how to find blends that match these targets. This design problem can become more complex and complicated with the infinite number of possible blending agents as it results to limitless possibility of blending candidate.

A systematic computer aided approach can efficiently solve this tailor-made green diesel blends design problem by providing a more efficient solution method than the iterative trial and error approach (Gani, 2004). This method had been widely applied to design skin-care cream (Cheng *et al.*, 2009), paint and insect repellent (Conte *et al.*, 2011), gasoline blends and lubricant base oils (Yunus *et al.*, 2014) etc. The computer aided technique is able to rapidly narrow down the search space of feasible green diesel blends so that the costly and time consuming experimental works can be done only on the selected promising candidates. This research is carried out to obtain an optimum tailor-made green diesel blends containing B5 palm oil biodiesel by using a decomposition-based computer-aided approach and subsequently, to validate the property and performance of the designed fuel blend using experimental works.

1.2 Problem Statement

Malaysia has launched the National Biofuel Policy in year 2006 to commercialize palm oil biodiesel and to promote the use, export and research on biodiesel and other renewable fuel from biomass, mainly focusing on lignocellulosic

biomass (Chin, 2011). B5 palm oil biodiesel (B5) mandate was launched in Malaysia since 2011 by region (started from the central regions: Kuala Lumpur, Selangor, Putrajaya and Melaka) and it was fully implemented nationwide on July, 2014. Meanwhile, Malaysia prospected to achieve Euro 5 emission standard diesel fuel in year 2020 in order to cut off 40 % carbon footprint in year 2020 compared to year 2005 (Begum and Pereira, 2011). Unfortunately, the use of biodiesel always leads to higher NO_x emissions and this increment will become significant when more biodiesel is blended with petrodiesel (Man *et al.*, 2016). Furthermore, highly relying on edible palm oil-based biodiesel can induce the conflict between food and fuel and raising the food (palm oil) price. In order to get an alternative diesel fuel blend with greener emissions and higher portion of biofuel/bio-chemical, it is essential that other lignocellulosic bio-chemicals with excellent fuel and combustion characteristics (e.g. high oxygen content and cetane number) to be introduced into B5.

The main concern related to the tailor-made green diesel blend design problem is how to find the suitable blending agent (biofuel/bio-chemicals) and how to find the blends with desired target properties. Trial and error is a traditional experimental method used to solve a blending design problem. This method is unfavorable as numerous repeats and varied attempts are needed and continued until the problem is successfully solved. It will become more troublesome and expensive when a blending design problem has enormous possible blend candidates. Hence, a systematic computer aided tailor-made green diesel blend design algorithm is essential to solve the blending design problem. Ariffin Kashinath et al. (2012) computationally design petrodiesel-ethanol, butanol and/or butyl levulinate blends based on linear property models of density, viscosity, distillation temperature and cetane number without performing experimental validation. Hence, the accuracy of the design method presented by Ariffin Kashinath et al. (2012) is unknown. Hashim *et al.* (2016) extend the works presented by Ariffin Kashinath et al. (2012) by introducing experimental validation. A more comprehensive computer-aided blended product design algorithm is introduced by Yunus et al. (2014). This method was used to design gasoline and lubricant blends from molecular level up to the end product; but, no experimental validation is performed and this generic method is not used to

design green diesel blends. None of the foregoing methods consider fuel additive (e.g. cetane enhancer) to enhance the design blends in their design algorithm whereas it could be very important as some of the fuel properties are difficult to attain by solely using blending agent/s (bio-chemical/s). In addition, another important safety related fuel properties: flash point is not involved in the foregoing studies in the computer-aided design stage.

Flash point of a liquid petroleum product is defined as the lowest temperature at which the fuel must be heated to produce sufficient vapors that ignite spontaneously in the present of a flame (Crowl and Louvar, 2002). Flash point is rarely been considered in the early green diesel blend design stage as it has no directly effects on engine performance and combustion. However, it is a very important information related to handling safety, such as distribution operation and storage condition (Dharma *et al.*, 2016). On the contrary to the lighter petrol fuel, in which its flash point is much lower than 0 ˚C (- 43˚C) and it is always too rich to ignite under atmosphere when contact to a flame as its vapor concentration in air is above the upper flammable limit of gasoline, the flash point of the heavier diesel fuel must be high enough to prevent fire accident. Table 1.2 showed the flash point standard values of diesel in few countries. Overall, the flash point values are above 50 ˚C, except in India. As reported by (Thilagen and Gayathri, 2014), numerous fire accidents occurred in India due to the low flash point of diesel fuel as it can easily cause explosion of diesel tank when transport vehicles collided. On the other hand, Guibet and Faure-Birchem (1999) comments that blending gasoline to petrodiesel fuel should be prohibited as unacceptable flash point reduction happened and causing gasoline-petrodiesel blend to be highly flammable under atmosphere. Hence, it is important to have diesel fuel with high flash point and it should not be omitted when designing green diesel blends.

Table 1.2: The flash point standard limits in various countries (Thilagen and Gayathri, 2014)

Country	Diesel flash point, ˚C
China	66
Pakistan	66
Australia	61
Malaysia	60
Norway	60
Srilanka	60
Germany	56
U.K	56
Finland	55
Italy	55
Netherlands	55
U.S.A	54
Thailand	52
Ireland	51
Japan	50
India	35

An accurate flash point prediction model is needed to design green diesel blends containing B5 with safe handling characteristics. Liaw model (Liaw *et al.*, 2002) is a reliable flash point prediction model to predict the flash point of non-ideal mixture. It has been widely applied to predict the flash point of binary (Liaw *et al.*, 2002) or binary aqueous (Liaw and Chiu, 2003) mixtures; ternary (Liaw *et al.*, 2004) or ternary aqueous (Liaw and Chiu, 2006) mixtures; biodiesel-ethanol blends (Guo *et al.*, 2009a, Khalili and Zarringhalam Moghaddam, 2011); and varied partially miscible mixtures (Liaw *et al.*, 2008a, Liaw *et al.*, 2008b, Liaw *et al.*, 2009, Liaw *et al.*, 2010). The accuracy of Liaw model is highly dependent to the activity coefficient. As the molecular binary interaction parameters that are needed for e.g. Wilson, NRTL and UNIQUAC activity coefficient models are always not available for many compounds; UNIFAC-based model is preferred. Only group-group interaction parameters, which are widely available and updated from time to time, are needed to calculate the activity coefficient using UNIFAC-based model. Hence, UNIFAC-based Liaw model shows great potential to predict the flash point for varied tailor-made green diesel blends that contain B5. Unfortunately, the accuracy of the UNIFAC-based Liaw model haven't been validated for green diesel blends containing B5 and its accuracy is needed to verify in order to have a reliable green diesel blends design algorithm.

In conclusion, there is a need to develop a comprehensive systematic computer-aided tailor-made green diesel blend design algorithm to obtain green diesel blends that match the desired target fuel properties and with lower emissions than B5. The design algorithm must able to computationally design the optimum green diesel blend by finding the suitable blending agent to blend with B5 in order to look at every single potential binary and ternary blend candidates (by pairing each generated blending agent with B5); and considering fuel additives to further enhance the design blends. Experimental validation must be performed at the end of the design algorithm to study the optimum blends experimentally for further development. In addition, the prediction accuracy of the flash point prediction model: UNIFAC-based Liaw model for the green diesel blend containing B5 need to be checked and improved when needed.

1.3 Research Objectives

The aim of this research is to propose an integrated systematic computer-aided framework with experimental approach to obtain tailor-made green diesel. To achieve this goal, the sub-objectives are listed as follows:

1. To develop a systematic computer-aided tailor-made green diesel blend design algorithm for tailor-made green diesel blend design problem.
2. To improve flash point prediction model based on the Liaw model for green diesel fuel blend.
3. To validate the physicochemical properties and determine engine performances and emissions of the designed optimum green diesel blends using experimental works.

1.4 Research Scopes

In order to attain the aforementioned objectives, the research scopes have to include the followings:

1. Retrieve the required data (e.g. fuel properties) from the database of the computer tool: ICAS version 17.0 or literature, if available.
2. Generate the possible blends candidates (with ester, ether and alcohol) using computer-aided molecular design tools: ICAS-ProCAMD.
3. Optimize the tailor-made green diesel blends containing B5 with ester/ether/alcohol using simulator-optimizer/calculation of MATLAB software.
4. Verify and improve the flash point prediction accuracy of the Liaw model using UNIFAC type models for B5-ester/ether/alcohol blend, and embed the improved flash point prediction model to optimize the green diesel blends.
5. Perform experimental works to validate the fuel properties and measure the engine performances and emissions of the design diesel blends in a four-stroke diesel engine.

1.5 Research Contribution

The main contribution of this research is an improved model-based method for tailor-made green diesel blends design as compared to the traditional trial and error experimental approach. The specific research contributions are listed as follows:

1. Contribution 1: A new systematic tailor-made green diesel blends design algorithm for tailor-made green diesel blend design.
2. Contribution 2: Improved flash point prediction model for tailor-made green diesel blends contains B5.
3. Contribution 3: New tailor-made green diesel blends, which are safer for environment and humans with less pollutants and green house gasses release as compared to the conventional B5, are obtained.

A substantial part of the results obtained in this research is published in international journals and presented in international conferences. The list of research publications and attended conferences can be found in Appendix A.

1.6 Thesis Outline

This thesis is divided into seven chapters. Chapter 1 introduces the research background, problem statement, research objectives, scopes and contributions of the presented study. A comprehensive literature review is provided in Chapter 2. Chapter 3 describes the research methodology that comprises of the systematic computer aided tailor-made green diesel blend design algorithm, improvement of flash point prediction accuracy for tailor-made green diesel blends containing B5 and experimental validation and measure of the physicochemical properties and engine performances and emissions of the optimum green diesel blends. Chapter 4 describes the results obtained for flash point model improvement while the results obtained for green diesel blend optimization using the developed design algorithm is presented in Chapter 5. Subsequently, the experimental results of the physicochemical properties and engine performances and emissions of the optimum green diesel blends are discussed in Chapter 6. Finally, Chapter 7 summarizes the main findings obtained in this research.

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