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Computational and Experimental Investigations on Tailor-made Biofuel Blend Properties

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Abstract

In regards to sustainability and environmental reasons, biomass based biofuel has emerged as promising candidates amongst other alternative vehicular fuel options. Feedstock selection contributes to diverse biofuel blend components. Through computational product design, potential candidates can be generated and screened from a large pool of fuel blends. Computational approaches minimize the search region and assist focused experimental work as conventional experimental methods are exhaustive and time consuming. Fuel blend properties need to conform with fuel regulation standards in order to be accepted as a vehicular fuel option. This paper compares computationally generated tailor-made biofuel blend properties with experimental methods. Results show notable errors for prediction of kinematic viscosity and distillation temperature of tailor-made biofuel blends associated with property models implemented in model formulation. Nonetheless, predicted and experimentally tested tailor-made biofuel blend properties complied with EN590 fuel regulation standard.

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Keywords: Tailor-made biofuel blends; Fuel properties; Computational approach.

1. Introduction

Alternative fuel options have pioneered the transportation sector for some time now owing to increased awareness on environmental effects, need for fuel sustainability, and finite supply of fossil fuels. Growing interest on biofuels as a vehicular fuel option is largely prompted by current researches centered on tapping potential of biomass as the primary energy source. Biofuels produced from biomass are categorized under second-generation biofuels which evade fuel versus food controversies.

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Malaysia is the world's second largest producers of palm oil generating surplus palm biomass waste that can be efficiently utilized for energy generation [1-3]. Biomass is composed of lipids and cellulosic materials. Depending on the type of feedstock, different conversion routes can be used to process biofuels using these components as starting materials [4-5]. Bioalcohols, biodiesel, bio-oils, bio-ethers, bio-esters, and synthetic hydrocarbons are basic building blocks for liquid biofuels. Among these, biodiesel and bioalcohols are widely commercialized with bio-esters emerging as an attractive fuel blend option. A mandate of five percent palm methyl ester (PME) blended in diesel, commonly known as B5 diesel, was introduced for commercial use in Malaysia in 2011. Studies are constantly conducted to improve and upgrade B5 diesel.

Fuel blend compositions gravely influence fuel properties [6-9]. Implementation of an alternative vehicular fuel option requires the fuel to meet specified properties that are parallel to conventional diesel. This facilitates existing engines to operate on the new fuels with little or no modification. Therefore, it is important to analyze physiochemical properties of fuel blends. The problem lies in identifying suitable blend compositions as the possibilities are endless. Experimental based, trial-and-error method is draining and consumes extensive resources to investigate properties for the wide range of fuel blend options. Computational approaches enable generation of potential fuel blend candidates in a fast and orderly manner while satisfying desired properties.

In this study, fuel blend candidates that satisfy a set of constraints for desired fuel properties were generated through computational approach. Termed as tailor-made biofuel blends, fuel blend components include B5 diesel, butanol, ethanol, and butyl levulinate. Physiochemical properties for the tailor-made biofuel blends were validated with experimental tests to ensure compliance with standard fuel regulations.

2. Computational Approach

2.1. Defining target properties

Essential attributes for selection of tailor-made biofuel blend candidates include environmental impact, product performance, safety factor, and economic value. These attributes are translated into target properties and target values. Physiochemical properties such as density, kinematic viscosity, cetane number, calorific value, and distillation temperature directly influence composition of fuel blends [7, 10-15]. Density and kinematic viscosity affects fuel atomization and spray pattern that controls combustion process in a diesel engine [7,10,14-15]. Fuel blends with higher cetane number is preferable as it enhances efficient fuel combustion [7]. Engine performances and exhaust emissions gravely depend on fuel combustion activities. Calorific value of a fuel is associated with the amount of power produced by fuel during combustion [13,15]. Denoga and Quiros reported weak correlations between distillation temperature and engine performances [16]. Nonetheless, distillation temperature is markedly an important safety measure as it signifies volatility of fuel.

2.2. Defining constraints

Tailor-made biofuel blends need to adhere with consistent fuel properties that are suitable for engine testing and applications. In absence of a standard for biofuel blends, the EN590 fuel regulation standard for conventional fuels was used as a baseline for comparison. Table 1 shows limit of desired target properties as in the fuel regulation standard. Limits for calorific value was estimated from calorific value of B5 diesel in Malaysia.

Table 1. Limits for target properties as in EN590 fuel regulation standard.

Fuel property	Units	Limits	
		Minimum	Maximum
Density at 15˚C	kg/m^3	820.0	845.0
Kinematic viscosity at 40˚C	cSt	2.0	4.5
Cetane number	-	46.0	-
Calorific value	MJ/kg	40.0[a]	-
Distillation temperature	˚C	-	360.0

[a]Estimated value (10% from calorific value of B5 diesel)

2.3. Selection of fuel blend components

Alcohols are among the widely investigated alternative fuel blend option. Incorporating alcohols in biofuel blending reduces viscosity and density of the blends [6,8]. In this study, ethanol and butanol were selected as fuel blend components under the alcohols category. Butanol has relatively higher energy content and cetane number in comparison to ethanol [17-18]. However, ethanol is easily attainable and contributes to emission reductions. Butyl levulinate is a promising oxygenated fuel candidate that has gained abundant of attention lately [19-21]. Its high oxygen content promotes reduced emissions. Table 2 presents physiochemical properties for each blend component obtained through various literary sources [21-25].

Table 2. Physiochemical properties of tailor-made biofuel blend components.

Fuel property	B5 Diesel	Butanol	Ethanol	Butyl Levulinate
Density at 15˚C (kg/m^3)	854.70	810.00	789.00	974.00
Kinematic viscosity at 40˚C (cSt)	4.57	2.50	1.20	1.99
Cetane number	56.10	25.00	8.00	14.00
Calorific value (MJ/kg)	45.14	33.00	26.80	27.44
Distillation temperature (˚C)	364.70	118.00	78.00	232.00
Cost (RM/L)	2.76	42.00	44.00	400.00

2.4. Model Formulation and Fuel Blend Generation

Ultimate goal of this study is to generate various tailor-made biofuel blend candidates that satisfy specified constraints on fuel properties. The tailor-made biofuel blends were generated through a model-based approach using GAMS version 24.2 and modelled as the following Non-Linear Programming (NLP):

$$\min f(x) \quad \text{(objective function)} \tag{1}$$

$$g(x) = 0 \quad \text{(equality constraints)} \tag{2}$$

$$h(x) \leq 0 \quad \text{(inequality constraints)} \tag{3}$$

$$x \epsilon X \quad \text{(continuous variables)} \quad (4)$$

The model was optimized for minimum fuel blend cost by changing amount of butyl levulinate while satisfying equality and inequality constraints. Fuel regulation standard was used as constraints for the model. Inequality constraints consist of maximum and minimum allowable limit for fuel properties while volume balance was defined as equality constraint. Continuous variables, x, are real numbers that represent fuel blend components. Detailed formulation will be discussed in full paper.

Linear mixing rules such as Kay's mixing rule and Arrhenius equation were employed as blend property models to estimate fuel blend properties through additive functions of composition and pure component values [7,15,26-27]. Table 3 shows composition of tailor-made biofuel blends generated through GAMS solver.

Table 3. Generated tailor-made biofuel blend.

Tailor-made Biofuel Blend	Blend 1	Blend 2	Blend 3	Blend 4	Blend 5
Composition (volume %)					
B5 diesel	0.746	0.783	0.757	0.793	0.830
Butanol	0.244	0.217	0.123	0.097	0.070
Ethanol	-	-	0.100	0.100	0.100
Butyl levulinate	0.010	-	0.020	0.010	-
Total fuel blend cost (RM/L)	16.30	11.28	19.67	14.65	9.63

3. Experimental Testing

The tailor-made biofuel blend properties were tested according to the corresponding ASTM test method.

4. Results and Discussion

Fuel properties for tailor-made biofuel blends predicted through GAMS were validated with experimental testing. Fig. 1(a) shows density of tailor-made biofuel blends. Differences between the results were less than one percent and complied to EN590 fuel regulation standard limits for density. Fig. 1(b) illustrates results for kinematic viscosity. Significant discrepancy occurred with errors ranging from 25% to 39%. Arrhenius equation is incompatible to be used for prediction of kinematic viscosity of fuel blends in this study. Nonetheless, values obtained were between specified fuel standard.

Fig 2.(a) depicts cetane number of tailor-made biofuel blends. Except blend 2, values between predicted and actual cetane number for the blends vary considerably. Absolute error percentage was recorded at 6.78%. According to Christensen *et al*., presence of butyl levulinate in fuel blend reduce cetane number of the blend [21]. However, this claim is contradicting to the finding from this study as both predicted and tested fuel blend cetane number were higher than the EN590 minimum limit. Comparison between predicted and actual calorific value of the fuel blends are as presented in Fig. 2(b). Errors were recorded at less than ten percent.

Standard mixture property model for prediction of distillation temperature is absent in literature due to influencing factors from blend component's vapor pressure, atmospheric pressure, and composition of fuel [26]. Nonetheless, implementation of Kay's mixing rule was able to predict distillation temperatures

for tailor-made biofuel blends with error range between 9% to 15%. The predicted and tested values also conformed to the maximum limit of 360˚C as imposed by fuel regulations. Fig. 3 compares predicted and actual distillation temperature values for tailor-made biofuel blends.

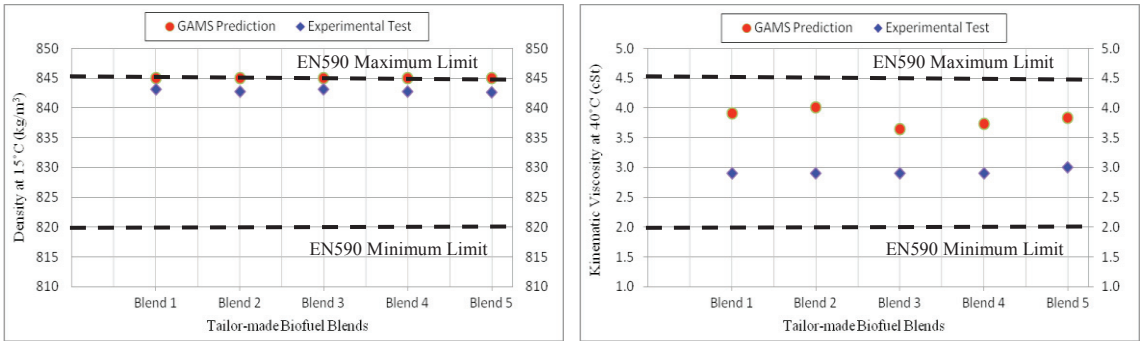

Fig. 1. (a) Density of tailor-made biofuel blends; (b) Kinematic viscosity of tailor-made biofuel blends.

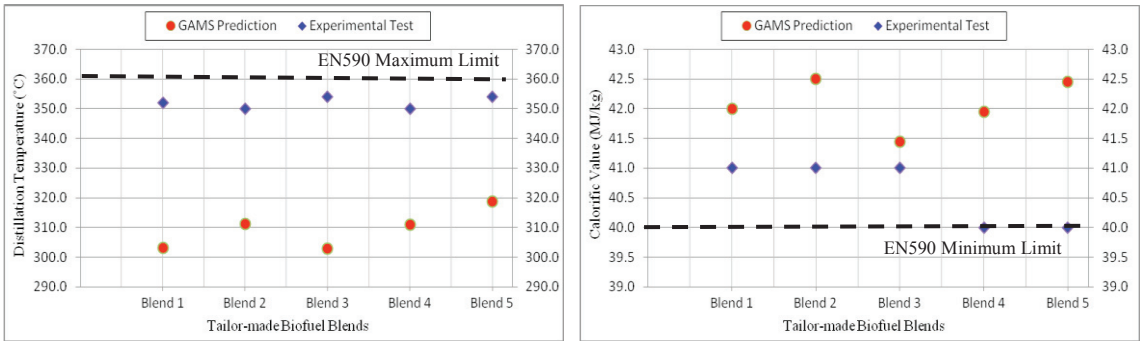

Fig. 2. (a) Cetane number of tailor-made biofuel blends; (b) Calorific value of tailor-made biofuel blends.

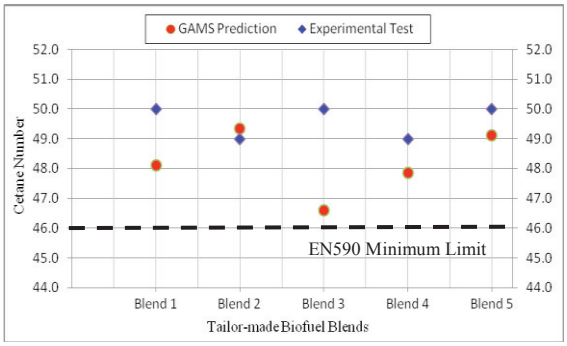

Fig. 3. Distillation temperature of tailor-made biofuel blends.

5. Conclusion and Recommendation

Computational approaches can be employed to assist in shrinking the search region for alternative fuel blends. In this study, GAMS solver was employed to generate various tailor-made biofuel blend candidates by changing amount of butyl levulinate and satisfying fuel property constraints. Linear mixing rules were incorporated into the solver to predict fuel blend properties. Predicted fuel properties were validated with experimental tests. Significant errors were observed for prediction of kinematic viscosity and distillation temperature. However, all investigated fuel properties complied to EN590 fuel regulation standard. Therefore, the set of fuel blends were deemed suitable for implementation as vehicular fuel option after further testing on engine performances and emissions have been conducted.

6. Copyright

Acknowledgements

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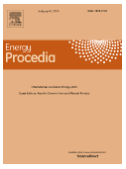
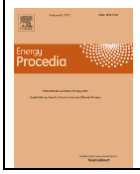


Biography

Haslenda Hashim is an Associate Professor in the Department of Chemical Engineering, Universiti Teknologi Malaysia. Her current research interests include modeling and optimization of green processes and product design, low carbon societies and process systems engineering.



Biography

Menaka Narayanasamy is a Masters student in the Faculty of Chemical Engineering, Universiti Teknologi Malaysia. Her current research interests include sustainable development with emphasis on design and modeling of alternative fuels.