Journal of Cleaner Production xxx (2016) 1–10

Contents lists available at ScienceDirect

Journal of Cleaner Production

journal homepage: www.elsevier.com/locate/jclepro

A cleaner and greener fuel: Biofuel blend formulation and emission assessment

Haslenda Hashim [a, b, *], Menaka Narayanasamy [a, b], Nor Alafiza Yunus [a, b], Lim Jeng Shiun [a, b], Zarina Ab Muis [a, b], Wai Shin Ho [a, b]

[a] *Process Systems Engineering Centre (PROSPECT), Research Institute for Sustainable Environment, Universiti Teknologi Malaysia (UTM), 81310, UTM Johor Bahru, Johor, Malaysia*
[b] *Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia (UTM), 81310, UTM Johor Bahru, Johor, Malaysia*

A R T I C L E I N F O

Article history:
Received 15 May 2016
Received in revised form
3 June 2016
Accepted 3 June 2016
Available online xxx

Keywords:
Biofuel
Fuel standard
Computational method
Experimental
Emission assessment

A B S T R A C T

Biofuel is an attractive vehicular fuel option for the transportation sector. Diverse biofuel blends can be produced from biomass. Complexity arises when optimum biofuel blends need to be designed to comply with fuel regulation standards as well as generate less emission. This paper discusses an integrated computational and experimental technique to design economically viable and environmentally friendly tailor-made biofuel blends from palm biomass that is abundant in Malaysia. An experimental based trial-and-error method is time consuming and uses up resources. Computational approaches adopt a systematic blend formulation methodology that assists focused experimental work. The biofuel design problem has been formulated as a Non-Linear Program to satisfy specified target properties such as density, kinematic viscosity, cetane number, gross calorific value, distillation temperature, and sulphur content. Target properties predicted through mixture property models were experimentally validated according to ASTM standard test methods. Five optimum tailor-made biofuel blend formulations were generated based on cost, gross calorific value and emission limitations. The result indicates that biofuel blends with butyl levulinate could increase the price of biofuel up to 80% from the retail price of B5 diesel. However, cleaner biofuel with less cost and highest calorific value can be achieved for biofuel blends that contain B5 diesel, butanol and ethanol. The application of this model yields about 26% CO_2 emission reduction and about 22% less sulphur content as well as comply with the EN590 fuel regulation standard.

1. Introduction

Government regulations, stringent laws on greenhouse gas reductions, and unstable fuel prices have prompted the search for an alternative source of energy for the transportation sector. Biofuel is an environmentally friendly and renewable source that has been globally adopted in many countries with the support of government policies. The International Energy Agency, IEA (2013) predicted that around 27% of transportation fuel would be completely replaced by biofuels before the year 2050.

Malaysia is now part of a long list of countries that implement biofuel through the introduction of B5 diesel, which has a 5% blend of fatty acid methyl ester obtained from palm biomass. Generally, no modification is required on existing diesel engines and fuel systems that run on small amounts of biofuel blends. However, fuel blends need to adhere to the specified standards of conventional diesel.

Palm biodiesels are known to be highly viscous (Knothe, 2010) and emit increased levels of NO_x gases (Hamdan and Khalil, 2010) due to their fuel properties. Many effort aims to improve the properties of palm biodiesel through the combination of multiple biofuel sources. Iqbal et al. (2015) investigated the effects of blending palm biodiesel with coconut and jatropha biodiesel. It was found improved fuel blend properties and competitive engine performance with emission characteristics were observed in 20% jatropha-palm-coconut blend compared to conventional diesel. Sanjid et al. (2014) evaluated performance and emission characteristics of palm and jatropha blends. However, tests conducted at 5 vol% and 10 vol% blends recorded high fuel consumption and

* Corresponding author. Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia (UTM), 81310, UTM Johor Bahru, Johor, Malaysia.
E-mail address: haslenda@utm.my (H. Hashim).

http://dx.doi.org/10.1016/j.jclepro.2016.06.021
0959-6526/

nitrogen oxide emissions. Bio-alcohols are particularly useful when dealing with viscosity issues (Hussan et al., 2013). However, the low cetane number and calorific value of bio-alcohols require a combination of additives for better performance (Oguz et al., 2010).

The experimental based trial-and-error method is time consuming and uses up resources. A more efficient way is to use a model-based systematic methodology that employs computational approaches to narrow down the search region, followed with focused experimental work. The biofuel blends can be tailored to meet specific attributes, so as to be sustainable, economically sound, and environmentally friendly.

Systematic product design methodologies have recently expanded to include biofuel blend design. Hada et al. (2011) implemented chemometric techniques through a systematic method to identify molecular structures of biodiesel additives. The approach enabled the combination of property clustering techniques and group contribution methods in enhancing the design of molecular fragments that meet target properties. Simasatitkul et al. (2013) proposed systematic methodology to design, synthesis, and analysed an integration of market dynamics of biodiesel integrated with fatty alcohol and waste edible oil via an economical and operationally feasible process. Voll et al. (2012) combined a spatial partial equilibrium model of the wood market to predict price and demand for methyltetrahydrofuran profitability. Hechinger et al. (2012) proposed a framework that combined rigorous generation of molecular structures with stepwise reduction to simplify the screening and selection of potential biofuel candidates based on fuel properties. Phoon et al. (2015) implemented a decomposition-based computer-aided approach to identify feasible green diesel blend candidates that meet property constraints. Ulonska et al. (2015) presented a methodology to systematically screen fermentation products and processes that serve as a platform for biofuel production from lignocellulosic biomass. Manuel and Wolfgang (2016) developed a framework for model-based fuel design for the identification of biofuel components for use in spark-ignition and compression-ignition engines. Yunus et al. (2012) developed a computer-aided methodology to design gasoline with different types of blending agents. This work was later expanded upon to cover formulations of blended liquid mixtures with verification using rigorous models (Yunus et al., 2014). Kashinath et al. (2012) focused on the design an economical and environmental benign of tailor-made green diesel blends. However SO_2 emission has been neglected in the emission assessment. In addition, all the computational results obtained from related researches have not been validated by experimental work. This study aims to develop a new framework to design tailor-made biofuel blends via a computer-aided model-based approach with experimental validation. Experimental validation ensures the reliability of the designed biofuels, but has been frequently neglected except in a handful of studies. Fuel target properties were established according to the European Standard of fuel quality i.e. EN 590. The predicted biofuel properties were then validated through laboratory tests. The carbon dioxide emissions and fuel sulphur content of these biofuel blends are also discussed in this paper.

2. Methodology

Most studies on fuel blend design employs a forward approach that relies on property prediction from a set of fuel blend compositions. The model-based systematic methodology approach is based on the reverse of this concept. Systematic methodology in the design of the proposed fuel blend for this study follows the fundamental concept introduced by Gani (2004). The methodology is divided into four main tasks i.e. problem definition, identification of property models, generation of fuel blend formulation, and experimental validation of the formulated blend properties. Fig. 1 illustrates the tasks involved in designing tailor-made biofuel blends.

2.1. *Task 1: problem definition*

2.1.1. *Defining attributes of interest*

Defining the problem is key in constructing a systematic methodology for product design. Pertinent information could then deducted from problem definition. Attributes of interest in terms of designing tailor-made biofuel blends include cost, environmental impact, safety factor, and product performance. Generally, traits of product design encompass criteria such as economical viability and environmental friendliness without forsaking product quality. Nonetheless, the safety attribute is equally important, especially in the design of fuel blends. These attributes are then translated into target properties and target values. Table 1 summarises the list of target properties based on attributes of interest for the design of the tailor-made biofuel blends in this study.

2.1.2. *Defining target properties*

Important physiochemical properties that influence the fuel blends fraction include density (Benjumea et al., 2008), kinematic viscosity (Demirbas, 2008), cetane number (Varatharajan and Cheralathan, 2012), calorific value (Silitonga et al., 2013), and distillation temperature (Pandey et al., 2012). Fuel density and viscosity are important parameters that directly influence fuel atomisation (Jayed et al., 2011) and spray pattern (Al-Hamamre and Al-Salaymeh, 2014), which affects engine performance.

Cetane number characterises the tendency of fuel to combust under certain pressure and temperature on its own volition. Fuel with higher cetane number is more preferable as it ensures smooth engine operation and reduces exhaust emissions (Jayed et al., 2011). The calorific value of fuel is associated with the amount of power the fuel produces during combustion. Fuel with higher energy content will increase engine power output with less fuel consumption (Channiwala and Parikh, 2002). Distillation temperature represents the volatility of diesel, the readiness of liquid diesel change into vapor (Sajjad et al., 2014).

Denoga and Quiros (2004) observed a weak correlation between distillation temperature of fuels and engine performance parameters. However, fuel economy was shown to improve with lower distillation temperatures. Since distillation temperature signifies the volatility of fuel, this fuel property is markedly important as a safety measure. Maximum values for distillation temperature are commonly specified in fuel standards. The fuel sulphur content (Tan et al., 2009) is another property that is of great concern, as it greatly affects emissions from diesel engines and is a controlled factor in fuel standards (Tan et al., 2013).

2.1.3. *Defining constraints*

Novel biofuel blends need to adhere to consistent fuel properties to ensure suitability in engine testing and evaluation. In the absence of a standard for biofuel blends, both the American Society for Testing and Materials (ASTM) D975 and EN590 standards for conventional diesel fuels in the United States and Europe can be used as the baseline for biofuel blends containing up to 20% biodiesel (Geng et al., 2009).

In this study, the EN590 standard was employed as the baseline standard. Table 2 shows key fuel properties and their limits, as per the EN590 standard for fuels. Limits for calorific value are seldom specified in fuel standards. However, gauging the ability of power generation in alternative fuels is an important criterion. Thus, extra constraint in terms of fuel calorific value was set to design the tailor-made biofuel blends in this study. A 10% reduction from

Please cite this article in press as: Hashim, H., et al., A cleaner and greener fuel: Biofuel blend formulation and emission assessment, Journal of Cleaner Production (2016), http://dx.doi.org/10.1016/j.jclepro.2016.06.021