

Integrated linear programming and analytical hierarchy process method for diesel/biodiesel/butanol in reducing diesel emissions

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ABSTRACT

In this study, an attempt to obtain the optimal fuel blends consisting of diesel/biodiesel/alcohol, which satisfies the ASTM D975 and EN590, has been performed. Fuel blending is complicated due to the trade-offs concerning the various criteria. The Linear Programming fuel blending model only evaluates solutions concerning quantitative criteria with one single objective function. In fuel blending, qualitative criteria must be considered in making the final decision. A new methodological framework that integrates a two-stage product design optimisation model consisting of a Linear Programming (quantitative) and Analytical Hierarchy Process (AHP) (qualitative) is developed. The AHP was used to evaluate the criteria weight. Four criteria were implied in selecting the optimal blends, covering good performance, emissions limitations, cost-effectiveness, and safety trade-offs. Seven sub-criteria such as cetane number, the heat of vaporisation, oxygen content, sulphur content, CO₂ emissions, flash point, and feedstock cost are examined. Four alcohol oxygenates as alternatives to be selected methanol, ethanol, propanol, and butanol. The final AHP results depicted diesel/biodiesel/alcohol (Blend 1) comprising of 70% diesel, 20% biodiesel, 10% butanol as the optimal blends with higher performance (CN = 48.69), lowest cost (1.2 USD/L), and cleaner emission with 35% less sulphur concentration and 36% CO₂ emissions mitigated. The AHP results were then validated by employing Sensitivity Analysis for four scenarios by increasing 20% of the priority vector. The solution of the sensitivity analysis of weights levels indicates the acceptable possibility of achieving the objective/goal. Blend 1 (diesel/biodiesel/butanol) is the optimal blend, followed by Blend 4 (diesel/biodiesel/methanol), Blend 2 (diesel/biodiesel/propanol) and Blend 3 (diesel/biodiesel/ethanol). In conclusion, this proposed new framework provides the confident decision to select alcohol oxygenates for future fuel diesel/biodiesel/alcohol without an extensive experiment, thereby saving time and money and reducing harmful environmental impacts.

1. Introduction

Diesel generally emits the greenhouse gases (GHG) such as CO₂, anthropogenic NO_x along with SO_x, CO, volatile organic compounds (VOCs), and ozone (O₃). The US Energy Information Agency (EIA) forecasted that global CO₂ emissions would increase by 43% by 2035. The transportation sector is projected to contribute about 24% of world CO₂ emissions in 2035, as shown in Fig. 1. Road transportation emits 80% of the light, and heavy transportation's total CO₂ contribution, followed by aviation at 13%, maritime shipping at 7%, and rail at 0.5%.

Several alternative fuels, such as biofuels, can significantly reduce CO₂. Because CO₂ emissions significantly increased, transport decarbonisation is necessary to promote and accelerate a low carbon environment to combat climate change. One of the practical solutions available today to decrease CO₂ emissions in transport is sustainable alternative biofuels such as biodiesel and bioalcohol. About 4.8 Gt of oil equivalent biomass converted to biofuel in 2050 (Ul Hai et al., 2019). Low carbon-emissions fuels and zero sulphur content biofuels such as biodiesel and bioalcohol can mark a substantial reduction of CO₂. However, to get the overall picture is needed to analyse the total

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Greenhouse Gases (GHG) footprint (Čuček et al., 2012).

Numerous researchers recently claimed that biodiesel obtained greater attention in the automotive industry as a promising alternative fuel because the physicochemical properties of biodiesel are extremely relative to diesel (Razak et al., 2017). Biodiesel permits a superior technological advantage over diesel, such as having a higher cetane number (CN), ultra-low sulphur, and aromatics, and also containing 10%–11% more oxygen content (OC) (Hasan and Rahman, 2017). These advantages are resulting in a substantial reduction of regulated pollution such as unburned hydrocarbons (HC), carbon monoxide (CO), and particulate matter (PM), and polycyclic aromatic hydrocarbons (PAHs) (Fanick and Kroll, 2018) but increased nitrogen oxides (NO_x) emissions (Killol et al., 2019).

Adding biodiesel at a higher amount in the diesel could emit higher NO_x due to increased OC and higher combustion temperature (Hagos et al., 2017). Increasing biodiesel content B0 to B100 can significantly reduce HC, CO, and PM emissions but increase NO_x emissions slightly (Thangaraja et al., 2016). PM and NO_x are indirectly proportional, with a 7%–15% increase in NO_x (Razak et al., 2021) during a 50%–70% decrease for PM, CO, and HC emissions. The higher OC in biodiesel prompts higher combustion temperatures, resulting in higher NO_x emissions. Similar results are consistent with Ruhul et al. (2017), who claimed that diesel blended with 12% Karanja biodiesel increased the NO_x emission up to 4.64%.

Some modifications are required for the binary diesel/biodiesel blends fuel to reduce NO_x and other harmful pollutants without deteriorating the engine performance (Sorate and Bhale, 2015). Alcohol oxygenates have been explored to reduce NO_x and other pollutants emissions by improving combustion chemistry (Silitonga et al., 2018) without significantly reducing the engine power. The oxygenates, also known as fuel borne, can further enhance the fuel properties and upgrade the engine performance caused by their thermochemical properties (Zhang and Balasubramanian, 2018). Oxygenates generally contain hydrogen, carbon, and oxygen.

A wheel-to-wheel analysis revealed that oxygenates could reduce sulphur, PM, and CO₂ significantly without affecting the engine performance as reported in (Çelebi and Aydın, 2018) and slightly NO_x formation (Xu et al., 2020). Wei et al. (2018) also supported this approach, which claimed that diesel/biodiesel/butanol at a maximum of 15% by volume of butanol could also successfully cut down 30% of NO_x formation and 20% CO₂ emissions. Diesel/biodiesel/alcohol is called tailor-made clean diesel (Razak et al., 2019).

In contrast to biodiesel, clean diesel is a green renewable diesel comprising biodiesel (esters) and oxygenates (alcohol), as shown in Fig. 2. The clean diesel comprises long-chain hydrocarbons ranging from C₁₅–C₂₁, a similar molecular structure to diesel. It has been considered a premium diesel due to a better PM, NO_x, CO₂, and other exhaust emissions.

Most biofuel formulation studies only concentrate on the traditional trial-and-error experimental fuel blending. This traditional blending is time-consuming, not economically viable, and environmentally friendly

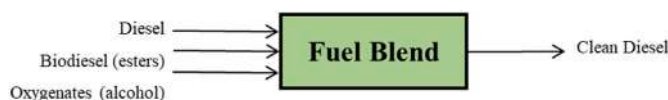


Fig. 2. Fuel blending of clean diesel.

as numerous attempts are required. The best strategy to meet these challenges while remaining profitable and maintaining sustainable growth, a computer-aided product design via model-based optimisation with specified property constraints (Hashim et al., 2017). The expensive experimental-based method with numerous candidates and alternatives is reserved only to verify the most promising candidates. Model-based product design is a systematic methodology that can design a higher added value product with enhanced product qualities and promote an efficient alternative (Zhang et al., 2020).

2. MCDM analysis – linear programming and AHP

A model-based product design can be achieved via Linear Programming. Linear Programming (LP) is one of the most straightforward Multi-Objective Decision Making (MODM) methods. There are three major components of LP: decision variables, objective function, and constraints (mathematical inequalities or equalities). Linear Programming is the most straightforward constrained optimisation problem in selecting the best and optimal solution by minimising or maximising a linear function of the decision variables. The linear maximised or minimised linear function is called the objective function. The main drawback of LP is that it can only optimise a single objective function.

For example, MODM optimisation was employed by (Yunus et al., 2014) for gasoline blending (Phoon et al., 2015), for diesel blending (Razak et al., 2021), for alcohol biofuel blending (Kalakul et al., 2018) for lubricant blending, and (Hashim et al., 2017) for alcohol and ether biofuel blending.

Fuel blending features the interactions of the fuel physicochemical properties to the three sustainability dynamic factors include economic, technological, and environmental indicators (Dahmen and Marquardt, 2017). All these three variables can be defined as quantitative parameters.

Fuel blending focuses on the tailor-made fuel formulation’s physical and thermochemical properties for the optimal fuel blends (Rodríguez-Fernández et al., 2019). Prior studies on fuel blending primarily focus on feasible quantitative criteria using MODM such as Linear Programming. The target is to maximise fuel efficiency and minimise cost and/or emissions impacts.

Linear Programming (LP) model evaluates solutions for quantitative merit with one single objective function. In fuel blending, qualitative factors must also be considered when making the final decision. Qualitative factors are good at managing selection based on criteria weight without destroying complexity. Complex fuel blending scenarios needed to resort to a sophisticated procedure, multi-criteria decision making

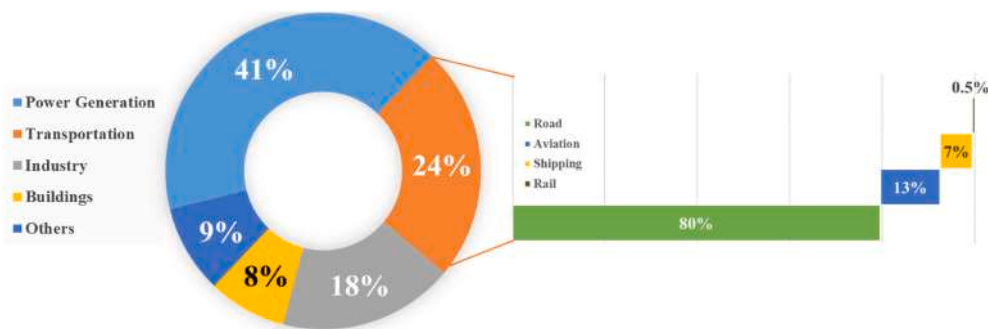


Fig. 1. Forecasted world CO₂ emissions in 2035 (IEA, 2015).

(MCDM). The MCDM has multivariate heuristic methods to integrate the quantitative and qualitative decision strategy.

As a result, prior studies have relied extensively on hybrid MCDM methods, MODM and MADM for fuel blending. [Erdogan and Sayin \(2018\)](#) used a hybrid MCDM method to determine the most suitable biodiesel blended with diesel. Unlike traditional LP optimisation, MODM and MADM consider quantitative and qualitative values. Both merits can be synchronized for better results.

MCDM is categorised into two methods, Multi-Objective Decision Making (MODM) and Multi-Attributes Decision Making (MADM). MADM is associated with problems where the number of alternatives is predetermined. The scoring methods are the simplest MADM methods. AHP is the most applied MADM method due to its simple-to-understand and easy-to-convince method, providing a systematic linear hierarchical analysis ([Saaty, 2003](#)).

While MODM is a goal programming related to issues in which the alternatives have been non-predetermined and obtained clearly by solving mathematical models ([Zavadskas et al., 2019](#)). To conclude, MODM is a mathematical programming problem with multiple objective functions. In contrast, in MADM, several alternatives according to some criteria are selected and ranked.

Due to the fuel blending complexity, qualitative merit such as the operational limitations obtained by the practitioners should be considered. One operational limitation is safety measures for safe storage and handling. The AHP method was selected due to its simplicity and structure robustness, fast results, and low computational cost ([Saaty and Ergu, 2015](#)). Another reason for adopting AHP is that AHP provides reciprocal pairwise comparisons and has a multi-level hierarchical structure analysis to propose the best alternatives from a discrete set of feasible alternatives.

The optimal fuel blend of diesel/biodiesel and alcohol becomes critical from a sustainability perspective, especially given conflicting economic and environmental objectives. Factors such as fuel performance and safety further affect the selection ([Mandade and Shastri, 2019](#)). Fuel blending is often challenging because they contain an overwhelming boundary of design trade-offs such as quality and quantity merits of fuel performance, safety strategy, cost-effectiveness, and environmental issues.

The LP model only evaluates solutions concerning quantitative criteria with one single objective function. In fuel blending, qualitative factors must also be considered when making the final decision. As a result, the fuel blending optimisation problem should rely extensively on hybrid MCDM methods, quantitative (MODM), and qualitative (MADM) approaches.

Under similar hybrid methods, [Quiroz-Ramírez et al. \(2017\)](#) applied MODM and MADM to select the optimal blend of fermentable sugars for butanol production. A similar hybrid optimisation approach was used by ([Cambero and Sowlati, 2016](#)) to decide process synthesis and feedstock selection. [Sehatpour and Kazemi \(2018\)](#) applied Fuzzy and Goal Programming (GP) to predict an optimal fuel for light-duty vehicles in Iran.

[Sakthivel et al. \(2017\)](#) developed a novel hybrid MCDM method, Fuzzy TOPSIS, and the Fuzzy VIKOR approach to evaluate and select the optimal fuel biodiesel blend. [Erdogan et al. \(2020\)](#) adopted integrated Fuzzy AHP and Fuzzy MOORA methods to evaluate the effect of engine performance, emission, and combustion characteristics of thermal barrier coated diesel engines fuelled with a biodiesel blend. [Sakthivel et al. \(2019\)](#) implied FAHP-TOPSIS to select the optimum blends from the various alternative blends of fish oil and diesel.

2.1. Research novelty and objective

Limited study and attention are given in the literature to decisions on the fuel blends selection applying a hybrid method; Linear Programming (MODM) and AHP (MADM). There is no research from the literature dealing with the optimal fuel blend selection based on fuel performance, emissions, cost, and safety using a hybrid MCDM method; LP and AHP.

In this research work, LP generates feasible fuel blends formulation, namely as alternatives.

Meanwhile, AHP is used to determine the criteria weight for the deviation variables in LP. AHP scores the optimal fuel blends selection based on the pairwise criteria judgement. Most researchers delineate the feedstock selection for the fuel blending, not the fuel blending formulation. Fuel blends formulation via LP is important for generating alternative data sets for AHP selection. This work consequently addresses these research gaps.

The main novelty is that the new two-stage methodological framework is developed to systematically assess the optimal fuel blend selection using a hybrid MCDM optimisation model. An integrated LP diesel/biodiesel/butanol blend optimisation model and AHP for maximising fuel performance, maximising safety factors, minimising cost, and minimising emissions impact have been proposed simultaneously. Similar two-stage design optimisation for different targets/goals was found in reference ([Serna et al., 2016](#)) for sustainable chemical process route selection. This reference has also employed the integrated optimisation method ([Ren et al., 2018](#)) for agricultural water and land optimisation allocation under multiple uncertainties.

Additionally, the work considers Sensitivity Analysis to check how sensitive the actual ranking of the alternatives is to changes in the current weights of the decision criteria. The optimal diesel/biodiesel/alcohol fuel blends were selected confidently using AHP-Sensitivity Analysis. Notably, this systematic framework provides a practical decision-making platform for policymakers that simultaneously integrates the quantitative and qualitative concerns. The new two-stage optimisation model should increase the confidence in the decision and implement better solutions.

This study aims to propose a new and novel systematic methodological framework for fuel blending comprising a hybrid MCDM optimisation model. The LP (MODM) integrates with AHP (MADM). This integrated method is used to determine the best alcohol oxygenates blended with diesel/biodiesel to reduce emissions, maximising fuel performance and safety factors with minimal cost. The study was successfully achieved with the following objectives:

- i. Objective 1: To determine the most feasible clean diesel blend from diesel/biodiesel with alcohol oxygenates, satisfying the ASTM D975.
- ii. Objective 2: To obtain the optimal diesel/biodiesel/alcohol with lower exhaust emissions at a minimal cost.

2.2. Conceptual research design

A conceptual research design of this study, as shown in [Table 1](#) has been composed of a primary objective, fundamental concepts, critical and construct measurement, constraints and variables, and key results. The detailed framework has been presented in [Fig. 3](#).

3. Method

The novelty of the present work is integrating two-stages design optimisation for the generation of feasible diesel/biodiesel fuel blends with different alcohol oxygenates. In 1st stage, generating the feasible diesel/biodiesel/alcohol blends formulation that offers technically complies with the diesel standard (ASTM D975). Next, in the 2nd stage, employing the AHP approach to select and rank the optimal diesel/biodiesel/alcohol amongst the feasible blend candidates based on performance, emissions, safety, and cost criterion. The optimal diesel/biodiesel/alcohol blends results were validated using AHP-Sensitivity Analysis. The systematic and structured two-stage design optimisation methods, including the quantitative and qualitative merits as portrayed in [Fig. 3](#).

In [Fig. 3](#), the 1st stage indicates the feasible fuel blends formulation as Task 1 using LP. The single objective optimisation model concerns quantitative analysis only. The objective function maximizes the fuel

Table 1
Conceptual research design.

Research Objectives	Research Questions	Research Scopes and Key Results
<p>Objective 1: To determine the most feasible clean diesel blend from diesel/biodiesel with alcohol oxygenates, satisfy the ASTM D975.</p>	<ul style="list-style-type: none"> • What is the best blending ratio for clean diesel? • Which alcohol oxygenates can optimally blend with local diesel? • Lower alcohols (methanol, ethanol, or propanol) or higher alcohol (butanol) oxygenates for diesel/biodiesel? 	<p>Generating the most feasible clean diesel blend formulation by using GAMS, the global optimizer tool. The fuel properties of the feasible clean diesel blend have been benchmarked to the properties and standards of diesel in the market (ASTM D975). The product design optimisation model covers the process constraints, the product performance, and the price policies for the ingredients. Four (4) alcohol as oxygenates for diesel/biodiesel is studied: methanol, ethanol, propanol, and butanol. 20% Biodiesel as the primary reference and at least 1% Bioalcohol and 1% diesel must be present in the clean diesel blend formulation. <u>Key Result:</u> Higher alcohol blended (Butanol) with diesel/biodiesel is the best oxygenate, which yields higher engine performance and lower exhaust emissions.</p>
<p>Objective 2: To obtain the optimal diesel/biodiesel/alcohol with lower exhaust emissions at a minimal cost.</p>	<ul style="list-style-type: none"> • Which alcohol oxygenates can optimally blend with local diesel? • What are the attributes/factors that influence the most optimal fuel blends selection? 	<p>Generating the most feasible clean diesel blend formulation using Multi-Objective Decision-Making (MODM) and Multi-Attributes Decision Making (MADM) optimisation models. AHP model using ExpertChoice tool is needed to rank and determine the optimal fuel blends based on four attributes: i. performance, ii. environmental impact, iii. safety, iv. cost assessment. Linear Programming (LP) model evaluates solutions for quantitative merit with one single objective function. In fuel blending, qualitative factors must also be considered when making the final decision. It was necessary to resort to a sophisticated procedure for complex fuel blending scenarios, such as multi-criteria decision-making (MCDM). <u>Key Result:</u> 10% Butanol is the optimal blending ratio for diesel/biodiesel.</p>

performance governed by cetane number (CN). In the single objective function optimisation, the four feasible fuel blend candidates proposed as the outputs.

In the 2nd stage, AHP with multi-objective optimisation is implied to rank and select the optimal blends. For this selection, four criteria are inferred; performance, emissions, safety, and cost. Finally, the AHP-Sensitivity Analysis is accomplished to check the stability of the AHP results. This new and novel two-stage optimisation model for fuel blending selection framework is easy-to-understand and worth-to-implement procedures.

The contribution is grouped into three main tasks (Task 1-Task 3) to provide a comprehensive overview of this integrated MCDM optimisation model formulation for fuel blending. A two-stage decision analysis was developed to support the fuel blending framework for the first time, refer to Task 1 until Task 3. The feasible fuel blends formulation assessment using LP for Task 1. AHP optimisation for ranking and selecting the optimal fuel blend for Task 2 and Task 3.

Task 1, a model-based fuel blending design categorised into three dominant tasks (Task 1.1 to Task 1.3 in Fig. 3), was initially proposed (Yunus et al., 2014). For Task 1.1, the first step involves problem definition and specifying the target properties. The second step in Task 1.2 is developing the property model subject to target fuel properties, and the constraints are then generated. The third step in Task 1.3 is the generation of feasible fuel blends.

This formulation is to determine the feasible fuel blends that best match the target properties based on the performance criteria such as oxygen content (OC), cetane number (CN), and heat of vaporisation (HOV) in mitigating the hazardous pollutants, especially CO₂ emissions, and sulphur content, and simultaneously enhance engine performance without forsaking fuel quality.

For Task 2, the steps ultimately focus on the MADM method for selecting the optimal fuel blends from the feasible candidates obtained in Task 1. AHP tool is needed to rank and determine the optimal fuel blends based on performance, environmental impact, safety, and cost assessment. Finally, for Task 3, an AHP sensitivity analysis investigates the effect of fuel target properties before attributes adjustment to enhance the confidence in the results of optimisation models.

3.1. Task 1 fuel blending optimisation

3.1.1. Task 1.1 – Problem definition

a) Defining product demand

Fuel blends are obtained by mixing selected biofuels to best match the diesel target properties. The product demand is the key target for product design that can create interest for prospectus customers (Zhang et al., 2020). This first step identifies product needs and translates them into target physicochemical properties. The physicochemical properties, product target, and importance of target properties are in Table 1. The developed ontology encompasses product types, target properties, types of alcohol oxygenates for the clean diesel blends that satisfy the target properties. The attributes/criteria for fuel blend design formulation include performance, environmental impact, safety, and cost assessment.

The main objective of this work is to elucidate a new two-stage LP integrated with AHP to obtain the optimal tailor-made diesel/biodiesel/alcohol blends with good fuel performance and match the diesel standards; ASTM D975 (ASTM International, 2020) and European EN590 diesel standards (European Committee for Standardization 2014). Adding alcohol oxygenates to the diesel/biodiesel blend reduces diesel dependency, environmental impacts and enhances fuel properties (Nanthagopal et al., 2018).

b) Defining target properties

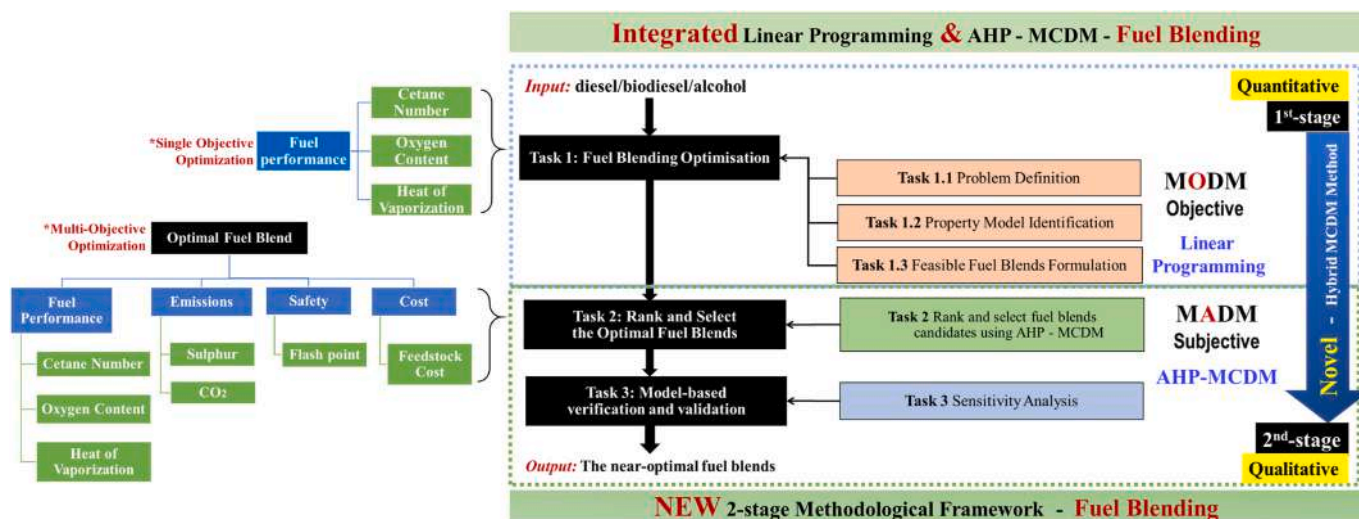


Fig. 3. The new systematic two-stage methodological framework for the tailor-made diesel/biodiesel/alcohol fuel blends.

To solve the blending problem, appropriate target properties are needed to get adequate and homogenised mixing. The important fuel target properties are cetane number (CN), oxygen content (OC), the heat of vaporisation (HOV), sulphur content, CO₂ emissions, flash point, and feedstock cost. Compared to pure component properties, the prediction of fuel blend target, particularly for biofuels (biodiesel and alcohol)

Table 2
List of product targets and their physicochemical properties.

Physicochemical Properties	Product target and their importance
Density	<ul style="list-style-type: none"> Represent the volumetric content of the fuel. The lower density fuel decreases fuel atomisation, leads to better combustion, and lowers NO_x and other harmful pollutants emissions (Qian et al., 2017).
Kinematic Viscosity	<ul style="list-style-type: none"> Ease of lubrication. Higher viscosity would impose additional loads on the injection system, which finally prompts poor combustion (Han et al., 2020).
Cetane Number, CN	<ul style="list-style-type: none"> Represent ignition quality and combustion intensity. The higher CN oxygenated fuel prompts shorter ignition delays, the less fuel evaporated, leading to a lower temperature, and consequently, NO_x and other harmful pollutants emissions reduced (Nabi et al., 2019).
Calorific Value, CV	<ul style="list-style-type: none"> Indicates the energy content of the fuel. The higher the CV, the more power output for the engine. Hence fuels with high calorific value are always preferred for automobiles (Wood et al., 2015).
The heat of vaporisation, HOV	<ul style="list-style-type: none"> The decisive influence of thermal NO_x formation. The higher the HOV, the lower the PM and NO_x formation due to a better evaporative cooling effect (Celebi and Aydin, 2018).
Sulphur Content	<ul style="list-style-type: none"> The tendency to form SO₂ and sulphate during combustion. The higher the sulphur, the higher the PM and NO_x emissions (Lapuerta et al., 2018).
Oxygen Content, OC	<ul style="list-style-type: none"> Promotes complete combustion of the fuel. The higher OC promotes cleaner emissions, reducing PM (Nabi et al., 2017) and NO_x emissions (Kumar and Saravanan, 2016).
Flash Point, FP	<ul style="list-style-type: none"> A safety measures for storage and transportation. The lowest temperature for fuel can vaporize to form an ignitable mixture in the air (flammability). Indicates the maximum temperature at which a fuel can be stored without serious hazard in a closed space (Schemme et al., 2017).
Feedstock cost, FC	<ul style="list-style-type: none"> Feedstock cost represents 75%–80% of the total cost (Zaharin et al., 2017). Mainly affect economic feasibility.

blended with diesel, is highly complex (Amin et al., 2016). Table 2 shows the fuel physicochemical properties and values obtained from the literature database.

Data from experimental tests do not cover the numerous fuel blends ratio at different test parameters. Therefore, the property model is required to predict the fuel blend properties. The alcohol oxygenates include ethanol, methanol, propanol, and butanol that can effectively reduce the viscosity (Imdadul et al., 2017) and NO_x and other harmful pollutants (Celebi and Aydin, 2019).

c) Defining the target property constraints

The constraints were set in lower and upper limits for every target property. Euro5 diesel specifications are the values limit and target fuel properties. The ASTM D975 and European EN590 (European Committee for Standardization) fuel standards for diesel have been accredited for the formulated clean diesel blend.

3.1.2. Task 1.2 – Property model identification

The required property model was retrieved from the linear mixing rule models. Fuel blend properties are more challenging to obtain than pure component properties. Experimental data do not examine the total blend fraction range at different test cases, and consequently, this inconsistency leads to imprecise and unreliable blending. Various fuel blending design problems requisite different sets of property models.

This work involves two blend property models: linear and nonlinear models. The Linear Kay’s and Arrhenius Mixing Rules were employed to predict the blend properties, and the target properties apply linear composition dependence. Both rules are critical in designing the optimal tailor-made clean diesel blend as they satisfy the thermodynamic properties of thermal fluids.

The first mixing rule is Kay’s Mixing Rule in Eq. (1) was applied to presume the density, calorific value (Amin et al., 2016), derived cetane number (Ariffin Kashinath et al., 2012), flash point (El-araby et al., 2018), oxygen content (Yunus et al., 2014), the heat of vaporisation, fuel sulphur content (Hashim et al., 2017), and total cost (Hashim et al., 2017) while an Arrhenius mixing rule as Eq. (2) is used for kinematic viscosity (Benjumea and Agudelo, 2008).

$$\zeta_B = \sum_i^n x_i \zeta_i \tag{1}$$

where ζ_B is a property of the blends, ζ_i is the corresponding property of pure i component and x_i is the fraction in volume or mass based on the

properties unit.

$$\ln\mu_{mix} = \sum_i^n x_i \ln\mu_i \tag{2}$$

where μ_i is the dynamic viscosity (kg/m.s) of pure i component and μ_{mix} is the dynamic viscosity of the blend (kg/m.s) and x_i is the fraction in volume or mass based on the properties unit.

Nonlinear models are identified to predict viscosity, density, and flash point. Those have been linearised to apply the simple linear mixing rules. Linearisation of viscosity and density with the relative error at 5% (Gülüm and Bilgin, 2017) while 10% relative error for flash point (El-araby et al., 2018). The differences show that these three properties linear models are not substantial, and linearisation was used.

The Linear Kay's and Arrhenius Mixing Rules are simple rules for predicting diesel/biodiesel blends (Chatrou et al., 2019). Both rules are essential in designing the fuel blends as they satisfy the thermodynamic properties of combustible fluids. Kay's mixing rule is used for predicting density (Amin et al., 2016), calorific value (Amin et al., 2016), derived cetane number (Kalakul et al., 2018), flash point (El-araby et al., 2018), oxygen content (Zhang et al., 2018), the heat of vaporisation (Yesilyurt et al., 2020), fuel sulphur content (Hashim et al., 2017), and cost (Hashim et al., 2017) while an Arrhenius mixing rule is used for kinematic viscosity (Hoang, 2018). Table 3 depicts the target properties models and constraints as tabulated in Eq. (3) to Eq. (14).

3.1.3. Task 1.3 – Feasible fuel blend optimisation

It is important to identify the suitable biofuels (biodiesel or bio-alcohol) to be blended with diesel. Several criteria were used to select biofuels candidates amongst the alcohol oxygenates. The model-based fuel blending was employed to generate the feasible fuel blend candidates that satisfy the target property value. All property models and target values were coded in MATLAB.

The clean diesel formulation is formulated as a linear problem (LP) and solved using MATLAB, modelled in a linear programming (*linprog*) solver. A similar model-based blend formulation method was also

employed for gasoline blending (Yunus et al., 2014), diesel blending (Phoon et al., 2015), alcohol biofuel blending (Razak et al., 2019), lubricant blending (Kalakul et al., 2018), and alcohol and ether biofuel blending (Hashim et al., 2017). All lower and upper limits inequalities were defined as equality constraints for this *linprog* problem.

The formulation of the model-based product design contains an objective function, variables, and constraints. Equality and inequality constraints for property and process models were defined. The linear property model constraints are as follows; cetane number (CN), the heat of vaporisation (HOV), oxygen content (OC), flash point (FP), fuel sulphur (S), CO₂ emissions, and feedstock cost (FC). The fuel property constraints used are set according to the Euro5 diesel standard. Each property has its role in producing an excellent clean diesel blend.

The objective function for the fuel blend design optimisation is set to maximise the cetane number. Ternary blend selected, alcohol, as an oxygenates, blended with diesel/biodiesel blend. The objective function is shown in Eq. (15). Several lists of feasible ternary diesel/biodiesel/alcohol blend candidates have been obtained.

$$F_{obj} = \max \sum_i^n CN_{mix} \tag{15}$$

where F_{obj} is the objective function and CN_{mix} represents the cetane number of fuel blends.

MATLAB gave four optimal blend compositions and property values with higher fuel performance (governed by CN). The results were generated within 0.015 s. The blend properties obtained were within the specified target values. The optimal fuel blends that satisfied all the constraints are then ranked according to the minimum difference cetane number, ΔCN_{mix} in the fuel blends over the CN of diesel. The subscript *mix* represents the ternary fuel blends (diesel/biodiesel/alcohol).

The alcohol oxygenates in the fuel blends designed in this study should have at least 1% by volume of alcohol and/or maximum at 20% by volume of biodiesel. This is because the higher oxygen content (OC) associated with the lower calorific value (CV) of alcohol oxygenates and higher viscosity of biodiesel leads to lower fuel economy (Nabi et al.,

Table 3
The fuel target properties and values.

Fuel Properties	Diesel	Biodiesel	Methanol	Ethanol	Propanol	Butanol
Chemical Formula	^a C ₁₄ H ₃₀	C ₁₂ – C ₂₂	CH ₃ OH	C ₂ H ₅ OH	C ₃ H ₇ OH	C ₄ H ₉ OH
Molecular Weight (g/mol)	^c 198.4	^d 293	^f 32.04	^j 46.07	ⁱ 60.09	ⁱ 74.12
Density at 15 °C (kg/m ³)	^a 839	^d 872	^f 791.3	^f 789	^g 803 at 25 °C	ⁱ 810
Kinematic Viscosity at 40 °C (mm ² /s)	^a 2.91	^d 4.56	^f 0.58	^f 1.1	^g 1.74	ⁱ 2.22
Cetane Number, CN	^a 49	^d 61	^f 5	^f 8	^g 12	ⁱ 17
Calorific Value, CV (MJ/kg)	^b 45.273	^d 39.8	^f 19.58	^f 27	^g 30.63	ⁱ 33.1
Heat of vaporisation, HOV (kJ/kg)	^a 274	^m 353	^l 1162.64	^l 918.42	^l 727.88	^l 581.4
Flash Point (° C)	^a 71.5	^d 184.5	^f 12	^f 17	^g 22	ⁱ 35
Self-Ignition Temperature (° C)	^l 254	^m 350	^l 463	^l 420	^l 350	^l 345
Oxygen Content, OC (mg/kg)	^o 0	^b 11	^f 49.93	^f 34.8	^j 26.62	ⁱ 21.58
Fuel Sulphur Content (mg/kg)	^o 0.26	^c 0	^h 0	^o 0	^g 0	^o 0
^o Feedstock Cost (USD/L)	^o 0.52	1	10	4	15	6

^a (Silitonga et al., 2013).

^b (Altaie et al., 2015).

^c (Hashim et al., 2017).

^d (Tutak et al., 2017).

^e (Agarwal, 2007).

^f (Kumar et al., 2016).

^g (Atmanli, 2016a).

^h (Sayin et al., 2010).

ⁱ (Atmanli, 2016b).

^j (Yilmaz and Atmanli, 2017).

^k (Benjumea and Agudelo, 2008).

^l (Rajesh Kumar and Saravanan, 2016).

^m (Subramani et al., 2020).

ⁿ (Javier et al., 2013).

^o The cost obtained from (Merck Sdn Bhd, 2021) includes pure alcohol's capital and production cost, transportation cost, and current sales profit in 2021.

^p ULSD No. 2 Diesel price in Malaysia in 2014 (Hussain et al., 2018).

2019). Further, alcohol oxygenates can absorb water, leading to metal corrosion and phase separation (ErdiwansyahMamat et al., 2019). Mahmudul et al. (2017) also claimed that higher alcohol content might lead to an explosion because alcohol is highly flammable and explosive, which needs extra care on the blending.

Furthermore, the ratio of biodiesel was maintained at a maximum of 20% by volume due to their shortcomings over diesel. Several studies have revealed that a higher amount of biodiesel may drive to higher viscosity, which causes clogged car filters and nozzles and consequently lowers energy content, hence degrading the engine power (Wan Ghazali et al., 2015). All limitations are designated as referring to ASTM D975 and EN590 standards.

The emission study is gaining importance since toxic gases affect the human respiratory system. The diesel engine combustion process consists of air, fuel, and heat-generating complete combustion and incomplete combustion products. CO, HC, NO_x, and smoke are considered products of incomplete combustion, while CO₂ and H₂O are the products of complete combustion. The more CO₂ emissions, the better the fuel oxidation. Instead of cleaner emission targets, CO₂ released amount (kg CO₂/L fuel) indicates the efficiency of the fuel to combust inside the combustion chamber.

The CO₂ emission factors (3.19 t CO₂/t diesel) were obtained from the Intergovernmental Panel of Climate Change (IPCC) technical report (IPCC, 2018) is shown in Eq. (16). The CO₂ emissions rely upon carbon contents, oxygen concentration, and the combustion efficiency of the fuel. Lacking oxygen can lead to incomplete combustion and release more CO emissions that react with other pollutants in the airborne to form potentially harmful ground-level ozone.

$$CO_2 = \frac{(3.19 \times \rho_{mixture} \times \nu_{D100})}{1,000} \quad (16)$$

where $\rho_{mixture}$ represents the density of the clean diesel blends in kg/m³; ν_{D100} represents volume fraction of diesel and CO₂ generated from fuel combustion expressed in kg CO₂/L.

3.2. Task 2 - rank and select the optimal fuel blends using AHP

The two last steps are key new fuel blend design methods for this work in the second stage. The feasible blend candidates proposed by the model were then optimised in the MCDM approach via AHP. Herein, a systematic fuel blend design optimisation with a decision support system was developed, and a hybrid MCDM method was integrated. This integration enhances the product design optimisation model by adding attributes to the confidence intervals of the optimisation. AHP also identifies where a reduction of uncertainties is necessary or beneficial. The optimal diesel/biodiesel/alcohol blend should have good performance as diesel, be safe to handle, emit cleaner emissions, and be economically viable.

Finally, sensitivity analysis will investigate the impact of fuel target properties before adjusting. Sensitivity analysis is important in model development, validation, and optimisation. Also, sensitivity analysis helps focus on the most sensitive fuel target properties for the model adjustment, avoids over-fitting, and reduces the effort of model adjustment. They allow system analysts to determine where to focus on system design to ensure robustness and accuracy across the range of inputs. Sensitivity analysis offers an interactive visual representation of the sensitivities of a single and a large set of properties. The results reveal a high degree of model stability (SuJeong and Ramírez-Gómez, 2017).

3.2.1. Analytical hierarchy process (AHP)

This fuel blends optimisation aims to identify and propose the optimal blend that can achieve the trade-offs between the cost and performance (mainly governed by CN). The LP model in the 1st stage, the optimisation model, only evaluates solutions concerning quantitative criteria with one single objective function. In fuel blending,

qualitative factors must also be considered when making the final decision.

Therefore, the model-based formulation was then evaluated in the 2nd stage by applying the most advanced technologies in the MCDM tool, the pairwise-comparison analytical hierarchy process (AHP) method using Expert Choice v11.5 software (ExpertChoice, 2009). The AHP offers user-friendly interfaces, automatic calculation of priority vectors and inconsistency, and multiple types of sensitivity analysis embedded with an interactive graphical dynamic solution. The main advantage of employing this software is reducing the processing time to generate the priority vectors and the sensitivity analysis for the optimal results (Ho and Ma, 2018).

The AHP includes constructing a hierarchical framework and pairwise comparison matrices, performing pairwise judgment, analysing the comparison results, and ranking the best alternative that best matches the product targets (Ahmed Ali et al., 2015). This ranking and selection are based on priority vector values and the pairwise seven-point judgment/criteria consistency ratio.

AHP is the manufacturing industry related to implementing corporate sustainable manufacturing practices is the most of the studies available in literature reviews. Dos Santos et al. (2019) claimed that only five published manuscripts are to be found embracing AHP for biofuel sustainability development from 2014 to 2018. For example, the AHP method was successfully practiced to eco-design biodiesel production in Vietnam (Dos Santos et al., 2019).

AHP is a structured and flexible decision-making process proceeding from the objective/goal to criteria to sub-criteria to the alternative courses of action in successive levels (Saaty, 2008). The hierarchical framework of the AHP method is widely employed for comparing the overall performance by selecting and prioritising the desirable product target (objective). Organising and analysing complex decisions of this structured approach require the following four systematic steps:

- a) Step 1 of AHP: Develop the AHP hierarchical framework and define the main objective of the analysis

The first stage of AHP implementation is developing the hierarchical framework, which clearly and systematically presents the relationship between the main objective/goal and the criteria and the alternatives. The AHP method construes the problem in three strategic stepwise covers a top-down and bottom-up approach (Russo and Camanho, 2015).

The first step is defining the target (objective/goal) that needs to be achieved. The second step is to model the problem and define the criteria to evaluate the solutions that emerge. The third step is the most important part of establishing priority amongst sub-criteria using the pairwise comparison judgment approach. At the bottom level, the determination of priorities for the alternatives relative to the main objective/goal.

Referring back to the previously mentioned concept, in this case study, four alcohol oxygenates, methanol, ethanol, propanol, and butanol, were used as an alternative for this AHP model. The optimal diesel/biodiesel/alcohol selection was defined as the design problem's objective/goal (Level 1). The critical four attributes/criteria of product targets (Level 2), such as fuel performance, emissions, safety, and cost, were specified, as shown in Fig. 4.

The sub-criteria in Level 3 are cetane number (CN), the heat of vaporisation (HOV), oxygen content (OC), flash point (FP), fuel sulphur (S) content, CO₂ emissions, and feedstock cost (FC) are depicted visually in Fig. 5. Level 4 characterises alternatives including Blend 1, Blend 2, Blend 3, and Blend 4 to be selected concerning the main objective/goal set in Level 1.

- b) Step 2 of AHP: Performing pairwise comparison judgment

The second stage in the AHP method performs a pairwise comparison

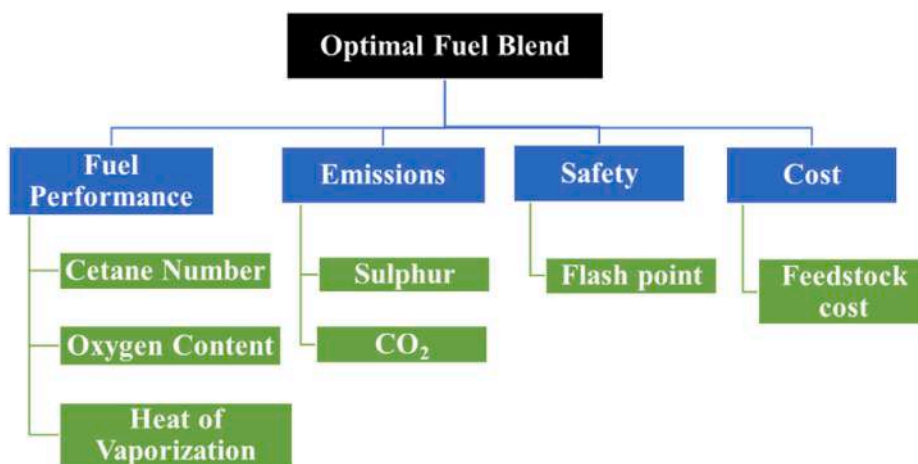


Fig. 4. Four criteria and seven sub-criteria of clean diesel blend product design evaluated in AHP optimisation model for the optimal blends.

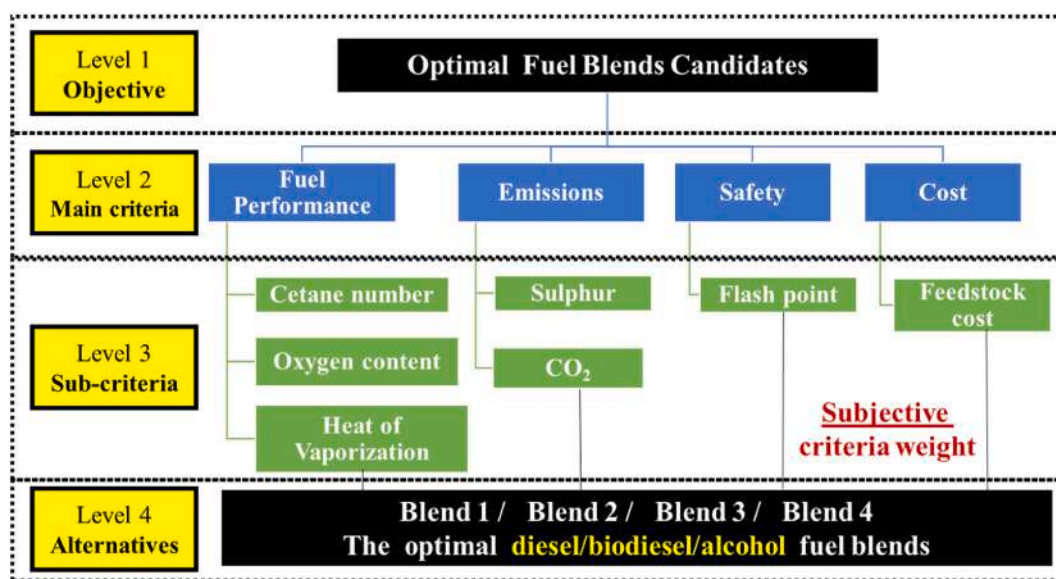


Fig. 5. The hierarchical framework in selecting the optimal clean diesel blend.

between the objective/goal and criteria. The individual elements are evaluated, and the consistency of the evaluation is checked. The pairwise comparison can be applied to determine which criteria are statistically significant. In this stage, the relative importance between the objective and the criteria, including the sub-criteria, are given a numerical value based on the ranking score for pairwise comparison.

The AHP method is the most frequently used criteria weighting method (MaiaAngelo and Lino Guimarães Marujo, 2020). Saaty (1990) uses the principal eigenvector of the positive pairwise comparison matrix to derive criteria weights from decision makers’ subjective judgment. In this work, the criteria weights have been determined using AHP. A subjective method is adopted to determine the criteria weights of economic, environmental, and technical attributes (safety and fuel performance).

The personal intuition of the decision-makers on the significance criteria for a specific decision-making process is adopted in the subjective model development. Several methods to obtain the criteria weights by applying a subjective approach can vary in the number of participants in the weighting process, the applied methods, and the forming of the final criteria weights. Subjective methods are principally based on pairwise comparisons of criteria (Pamučar et al., 2018).

c) Step 3 of AHP: Pairwise comparison evaluation by eigenvector

Subsequently, a pairwise comparison matrices using relative intensity is prepared for structured judgment. The Likert Scale method is a numerical scale for comparing two alternatives, as listed in Table 4. The AHP method is the most frequently used practice among all the subjective methods of assessing criteria weights (Vinogradova-Zinkevič et al., 2021). AHP quantifies the criteria weight in the form of a numerical basis. The criteria weight of each element determines its relative importance with the other elements of the hierarchy from Level 1 to Level 4.

The number of pairwise comparison evaluations depends on the criteria and is calculated using the $n(n-1)$ rule, where n is the number of criteria. It is necessary to assign relative weights to the criteria and evaluate the overall alternatives to get the best solution that matches their needs in the main objective/goal. The evaluation for the relative importance of the main objective/goal-criteria-alternatives are synthesised using the priority vector or eigenvector.

Saaty and Ergu (2015) obtained the priority vector by constructing pairwise comparison matrices (size $n \times n$) for each level, where n is the number of evaluation criteria considered. The priority value or eigenvector can be obtained by calculating the eigenvector of comparison

Table 4
Target properties models and constraints.

Attributes	Target properties	Linear Property Models	Lower Bound	Upper Bound	References	Reference for Test	Eqs.
Target property constraints							
Fuel performance	Kinematic Viscosity at 40 °C, η (mm ² /s)	$\ln \eta_{mix} = \sum_{i=1}^n x_i \cdot \ln \eta_i$	1.9	4.1	Hoang (2018)	ASTM D445	(3)
	Density at 15 °C, ρ (kg/m ³)	$\rho_{mix} = \sum_{i=1}^n x_i \cdot \rho_i$	810	845	Amin et al. (2016)	ASTM D1298	(4)
	Cetane Number, CN	$CN_{mix} = \sum_{i=1}^n x_i \cdot CN_i$	42	55	Kalakul et al. (2018)	ASTM D6890	(5)
	Calorific Value, CV (MJ/kg)	$CV_{mix} = \sum_{i=1}^n x_i \cdot CV_i$	43	-	Amin et al. (2016)	ASTM D240	(6)
	Heat of Vaporisation, HOV (kJ/kg)	$HOV_{mix} = \sum_{i=1}^n x_i \cdot HOV_i$	330	-	Yesilyurt et al. (2020)	ASTM D86	(7)
Safety concern	Flash Point, FP (°C)	$FP_{mix} = \sum_{i=1}^n x_i FP_i$	52	96	El-araby et al. (2018)	ASTM D93	(8)
Emissions impact	Oxygen Content, OC (mg/kg)	$OC_{mix} = \sum_{i=1}^n x_i \cdot OC_i$	2	20	Zhang et al. (2018)	ASTM D975	(9)
	Fuel Sulphur, S (mg/kg)	$S_{mix} = \sum_{i=1}^n x_i \cdot S_i$	-	10	Hashim et al. (2017)	ASTM D5453	(10)
Feedstock cost	Feedstock Cost, FC (USD/L)	$Cost_{mix} = \sum_{i=1}^n x_i \cdot FC_i$	-	5	Hashim et al. (2017)	-	(11)
Process model constraints							
Base fuel	Diesel ratio, x_D	$x_D \geq 0.01$	0.01	-	Razak et al. (2021)	-	(12)
Biodiesel	Biodiesel ratio, x_B	$x_B \geq 0.01$	0.01	0.2	Biodiesel limit to 20% for optimal results.		(13)
		$x_B \leq 0.2$					
Alcohol oxygenates	Cellulosic alcohol ratio, x_A	$x_A \geq 0.01$ $x_A \leq 0.2$	0.01	0.2	Maximum 20% alcohol has been limited due to lower CN and lower power output (Zaharin et al., 2017).		(14)

matrix A , as shown in Eq. (17).

$$A = (a_{ij})_{n \times n} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & 1 & \vdots & \\ a_{n1} & a_{n2} & \dots & 1 \end{bmatrix} \quad (17)$$

where $a_{ij} = k$ automatically implies that $a_{ji} = 1/k$ and $i, j = 1, \dots, n$ and $i \neq j$. The a_{ij} is the importance scale and n is the number of criteria.

d) Step 4 of AHP: Performing consistency analysis using Consistency Ratio

When many pairwise comparisons are performed, some inconsistencies may typically arise. Consistency Ratio (CR) plays a vital role in the hierarchical framework of AHP as CR can determine the consistency of pairwise comparison judgment. All comparisons between criteria and alternatives were analysed to determine the data consistency for each criterion. The priority value or eigenvector can be applied to compute Consistency Index (CI) and CR, as depicted in Eq. (18) and Eq. (19).

$$CI = \frac{\lambda_{max} - n}{n - 1} \quad (18)$$

$$CR = \left(\frac{CI}{RI} \right) 100\% \quad (19)$$

where n is the criterion, λ_{max} is the maximal eigenvalue of the comparison matrix, RI is the Random Index which depends on n values as tabulated in Table 5. The consistency rate (CR) should be less than 10%. The estimate is accepted if $CR \leq 10\%$ (Saaty, 2008).

The final stage in the AHP method is completing with sensitivity

Table 5
Importance scale for pairwise comparison analysis.

Relative Intensity	Definition (Example: a_{ij})
1	i and j are equally important
3	i is slightly more important than j
5	i is important than j
7	i is strongly more important than j
9	i is absolutely more important than j

analysis of the ranking of alternatives by using the Expert Choice v11.5 software program (ExpertChoice, 2009). Sensitivity analysis is adopted to validate the AHP results. This analysis is advantageous in understanding the effect of changing the weights of the main criteria on the ranking factors.

3.3. Task 3 - Sensitivity analysis

Sensitivity analysis is finally conducted to simulate the *What-If* simulation exercise to predict the outcome of a decision given a specific range of variables and conclude the robustness of the results. Moreover, it is a *Black Box Processes* that can help validate which factors are important and how changes in methods, models, or the values of variables affect the results.

A sensitivity analysis makes it possible to distinguish between high-leverage variables, whose values significantly impact the system behaviour, and low-leverage variables, whose values have minimal impact on the system. The overall AHP and sensitivity analysis have been presented in Fig. 6.

Four scenarios of varying the priority vector for the main criteria were performed in the sensitivity analysis using Expert Choice v11.5 software (ExpertChoice, 2009). The four scenarios in this study are performance (CN, OC, and HOV), environmental (sulphur content and CO₂ emission), safety (flash point), and economic (feedstock cost). Every main criterion for the four scenarios increases by 20%, and the results are analysed.

This section presents the results obtained from the proposed product design optimisation model for diesel/biodiesel/alcohol blends. Table 6 tabulates the optimal composition of four ternary clean diesel blends modelled in a linear programming (*linprog*) solver with linear objective function and continuous linear constraints (Yunus et al., 2014). All lower and upper limits inequalities were defined as equality constraints. The target property models, constraints, and target values were coded into MATLAB.

The optimal diesel/biodiesel/alcohol blends satisfied the desired Euro5 diesel target properties ASTM D975. Four types of primary alcohol have been considered for the blend design formulation: methanol, ethanol, propanol, and butanol. All proposed blends consist of 20% biodiesel and less than 20% alcohol. Maximum 20% alcohol has been limited because the higher alcohol content can lead to a lower fuel

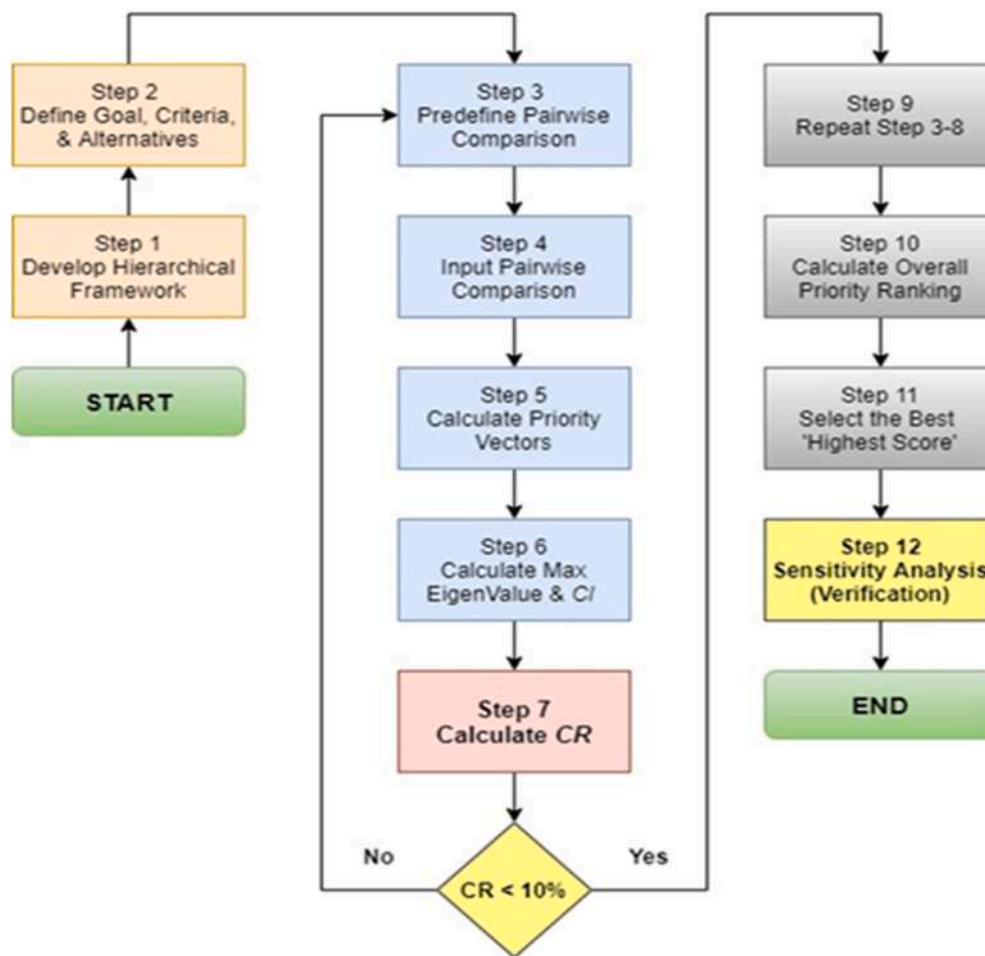


Fig. 6. AHP sensitivity analysis methodology.

Table 6
Random Index (RI) of random matrix (Raharjo and Endah, 2006).

n	2	3	4	5	6	7	8	9	10	11	12	13	14	15
RI	0.00	0.58	0.90	1.12	1.24	1.32	1.41	1.45	1.49	1.51	1.48	1.56	1.57	1.59

economy. The shorter combustion period of alcohol induces a decrease in the cooling effect, leading to higher NO_x emission (Zaharin et al., 2017).

Biodiesel is also limited to 20% due to higher viscosity and lower energy content, degrading engine power. Karavalakis et al. (2017) also reported that a low-level blend below B20 (20% biodiesel) is highly recommended to effectively curb CO₂, PM, and NO_x. B20 also performs similar horsepower, torque, and mileage as diesel (Alptekin et al., 2015) and will operate like diesel in any diesel engine without the need for modifications.

The tabulated results depict the CN for all four blends, Blend 1 until Blend 4, are approaching CN of diesel, CN = 49. These proposed blends showed that the diesel composition was reduced as the oxygenates increased. Blending diesel with biodiesel and alcohol is attractive since it substitutes 5%–15% of diesel fuel with biofuels, which can help to reduce the dependency on fossil fuels and reduce greenhouse gas emissions (Shahir et al., 2015).

Further analysis showed that the small volume of alcohol oxygenates in clean diesel blends could promote cleaner emissions, significantly reducing the harmful gases such as sulphur dioxide (SO₂) and the greenhouse gases, CO₂ (Kumar and Saravanan, 2016). The amount of CO₂ in fuel combustion emitted to the atmosphere was computed via Eq.

(16), as hypothesized (Ariffin Kashinath et al., 2012).

4. Results and discussion

Fig. 7 depicts the sulphur content and CO₂ emission reduction of the four blends compared to diesel. Diesel consists of 0.26 mg/kg sulphur concentration and 2.68 kg CO₂/L (Hashim et al., 2017). The fuel sulphur is burned and emitted as sulphates. The fuel sulphur content and aromatics hydrocarbon in diesel could increase the PM formation in the fuel blends. Notably, Lapuerta et al. (2017) claimed that fuel sulphur reduction promotes the reduction of PM formation by decreasing the particulate. The remarkable result from the plotted data is a significant reduction in sulphur content for about 35% and 36% CO₂ emissions abatement by Blend 1 (diesel/biodiesel/butanol).

Note that oxygenates like alcohol and biodiesel blended with diesel can boost fuel combustion to emit ultra-low sulphur (Natarajan et al., 2011) and lower PM (Jamrozik et al., 2018). Strong evidence of the findings is consistent with Çelebi and Aydın (2019). He claimed that biodiesel and alcohol's higher oxygen content (OC) leads to complete combustion and lower harmful gaseous emissions and smoke opacity.

Fig. 8 illustrates the trend of CN with the cost for all four blends in this case study. The CN increases with an increase in carbon alcohol.

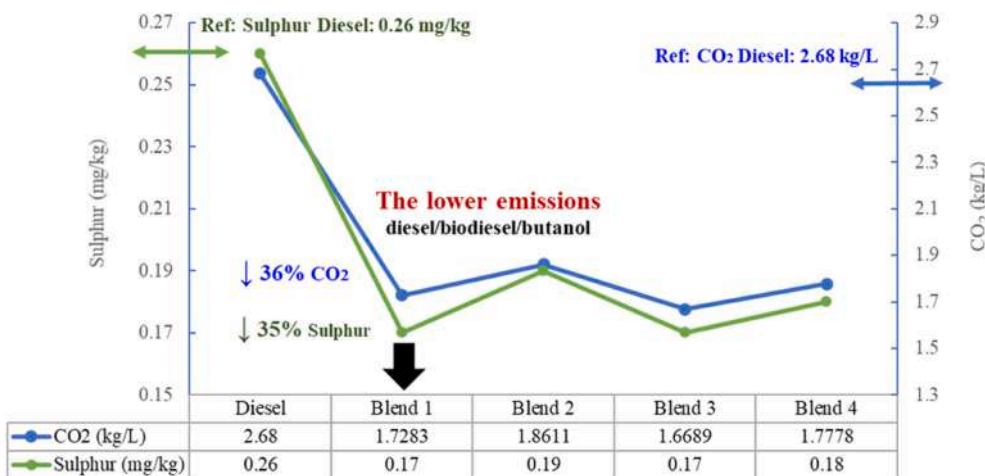


Fig. 7. Sulphur and CO₂ emissions reduction of diesel/biodiesel/alcohol blends.

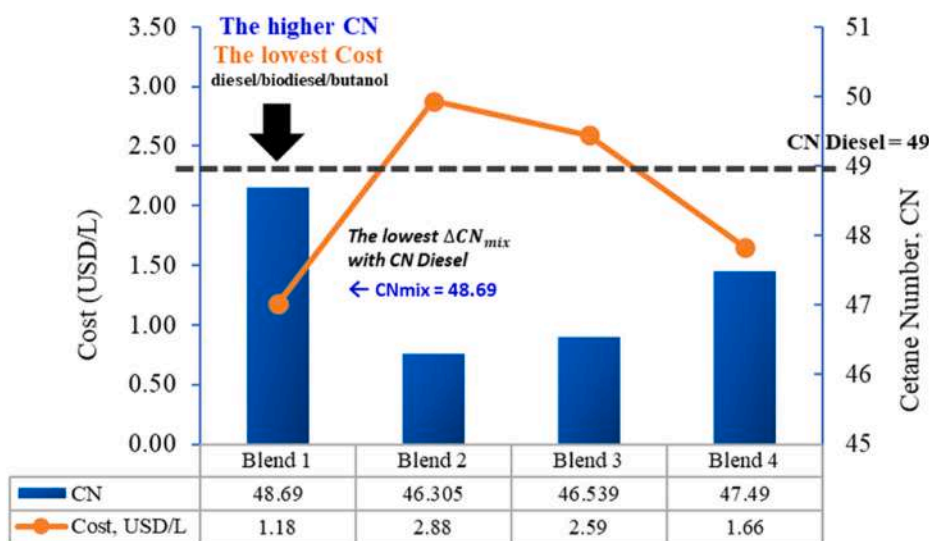


Fig. 8. CN and cost of diesel/biodiesel/alcohol blends.

This may be due to the increased CN of the lower alcohol (methanol, ethanol, propanol) to higher alcohol (butanol). It is apparent from this graph that CN for all four blends depicted is closing to 49, CN for diesel.

These results highlight that all four blends complied with ASTM D975. The CN experiences are the most critical fuel properties since the compression-ignition (CI) diesel engine relies on compression ignition (Emiro and Mehmet, 2018). CN indicates the ignition delay time that promotes combustion efficiency. The higher the CN, the shorter the ignition delay time, the better the combustion performance and cleaner emissions, and higher fuel economy.

4.1. Performing judgment using AHP pairwise comparison

AHP pairwise comparisons are used to prioritise criteria. Pairwise comparison is a numerical ranking process based on the ranking score comparing the relative importance, preference, or likelihood of the relative importance between the objective/goal and the criteria, including the sub-criteria. A pairwise comparison method is helpful in the MCDM context to determine the weighted ranking of alternatives or criteria/sub-criteria.

4.1.1. AHP pairwise comparison – graphical judgement

In this work, the ‘Graphical Judgement’ method in Expert Choice

v11.5 software program (ExpertChoice, 2009) is implied to evaluate the criteria weight. Two elements (criteria/sub-criteria) are compared to their parent elements with bar graphs. The lengths of the bars indicate the relative dominance of the elements. If they are of equal length, then the elements are equally important. If one bar is twice as long as the other, then it is twice as important. Relative dominance is also represented with a pie chart on the right side of the panel.

The numerical representations of the graphical judgments are displayed in the comparison matrix as numbers. If the row element (on the left) is preferred, the judgment is displayed in black. If the column element is chosen, the judgment is inverted and displayed in red. The final graphical judgment will be displayed as bar graphs that overlay the row elements depicted in Fig. 9.

Fig. 9 shows the pairwise comparison matrix of criteria, performance concerning the emissions. AHP performs a pairwise comparison to determine the most feasible ternary clean diesel blend to compare the objective/goal to the criteria, sub-criteria, and alternatives. The fuel properties depicted in Table 3 were used as a reference to assist the pairwise judgment. There are four alternatives concerning the four criteria: performance, emissions, safety, and cost.

The CN is a pervasive quality of the blended diesel with biofuels. The higher CN compensates significantly affect the fuel blends cost because alcohol is renewable, clean-burning fuel made from biological materials

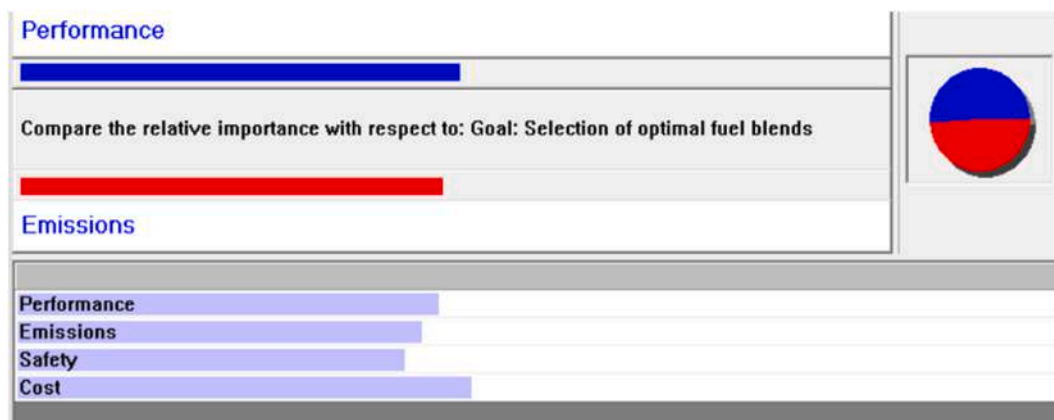


Fig. 9. The pairwise comparison matrix of criteria, performance concerning the emissions (ExpertChoice, 2009).

and renewable feedstock and may require a higher price for mass production. A pairwise judgment in AHP can be used to demonstrate the cost and performance trade-offs. The key desire is to get the best performance at the lowest price. As shown in Fig. 10, the CR is less than 10%, only 4%, meaning this pairwise judgment is acceptable and equitable.

Fig. 10 illustrates the priorities of four criteria to determine the optimal ternary clean diesel blends. The horizontal graphical bar demonstrates that cost (27.1%) is the highest priority, and the most crucial factor should be considered for clean diesel blends optimisation design. Fuel performance (25.3%) ranked as the second factor. The higher the CN, the excellent fuel quality can promote better fuel efficiency and complete combustion. Emissions (24.5%) ranked third in the selection, representing combustion efficiency. Safety (23.2%) ranked fourth in the priorities values.

Final AHP analysis, as shown in Fig. 11, concluded that Blend 1 (diesel/biodiesel/butanol) is the optimal diesel/biodiesel/alcohol blend. Butanol promotes better emissions, higher performance at a minimal cost, with the highest goal score, 25.4%. The second-ranked is Blend 2 (diesel/biodiesel/propanol) at 25.1%. Blend 4 consists of diesel/biodiesel/methanol ranked third at 25.1%, and Blend 3 (diesel/biodiesel/ethanol) ranked fourth at 24.3%. The overall inconsistency is 0.04.

4.2. Performance sensitivity analysis

The last step of the decision process is the sensitivity analysis, where the input data are slightly modified to observe the impact on the results. Sensitivity analysis has been conducted to verify the ranking and selection from the pairwise judgment performed (Chang et al., 2007). Sensitivity analysis is typically performed to check the robustness of the optimal solution. By performing Sensitivity Analysis, it can quickly be determined how a change in the importance of an objective would affect the choice alternatives.

This analysis was executed using Expert Choice v.11.5 software

(ExpertChoice, 2009). Parametric sensitivities can be determined from the LP and AHP results. The stability of the pairwise evaluation can be observed by changing the four criteria. The four criteria/scenarios are fuel performance, emissions, cost, and safety.

In this study, the priority vector of the four scenarios has been increased by 20%, and the overall rank change is shown in Fig. 12, Fig. 13, Fig. 14, and Fig. 15. A similar 20% change was found in (Mansor et al., 2013) in selecting a hybrid natural and glass fibers reinforced polymer composites material for automotive brake lever design. Mastura et al. (2017) reported that their Sensitivity Analysis results in selecting a hybrid bio-composite material for the automotive anti-roll bar are stable at 20% changes.

The Sensitivity Analysis results in this study 20% change for the criteria/scenarios are set in this study because the alternatives (methanol, ethanol, propanol, and butanol) do not change. The 20% changes are robust, indicating Blend 1 ranked top for all scenarios/criteria (fuel performance, emissions, safety, and cost). The results are consistent with data obtained in Prasad Bhuvanagiri et al. (2018), who identified that their results do not change significantly for the change at lower than 20%. Meanwhile, a significant change such as +30% and above resulted in inconsistent results and efficiency loss (Zondervan et al., 2015). This analysis is helpful because it improves the model's prediction by studying qualitatively and/or quantitatively how the model responds to the changes between variables.

Sensitivity analysis approaches measure the impact of change in input variables by understanding the phenomenon studied by analyzing interactions between variables (Mandal et al., 2012). Sensitivity analysis is performed using the following formula in Eq. (20).

$$S = \frac{\left(\frac{\partial x}{x}\right)}{\left(\frac{\partial p}{p}\right)} \tag{20}$$

where S is sensitivity, x is variable, and p is a parameter. ∂x and ∂p are changes of initial values of variables, parameters, and forcing functions.

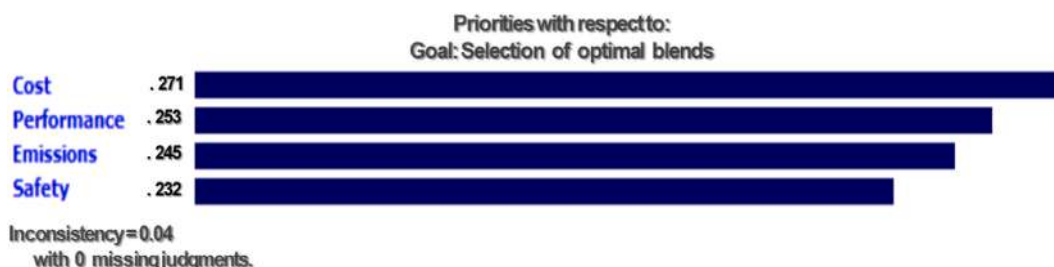


Fig. 10. The priorities ranking and scoring of the sub-criteria to the goal (ExpertChoice, 2009).

Synthesis with respect to: Goal: Selection of optimal blends

Overall Inconsistency: .00



Fig. 11. Overall results for diesel/biodiesel/alcohol fuel blends (ExpertChoice, 2009).

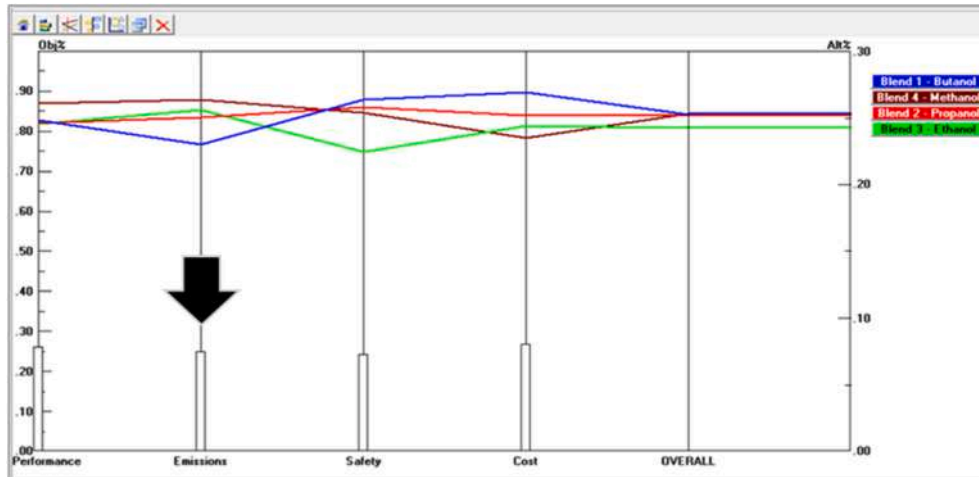


Fig. 12. Performance sensitivity graph of emissions concerning goal when the priority vector of environmental is increased by 20%.

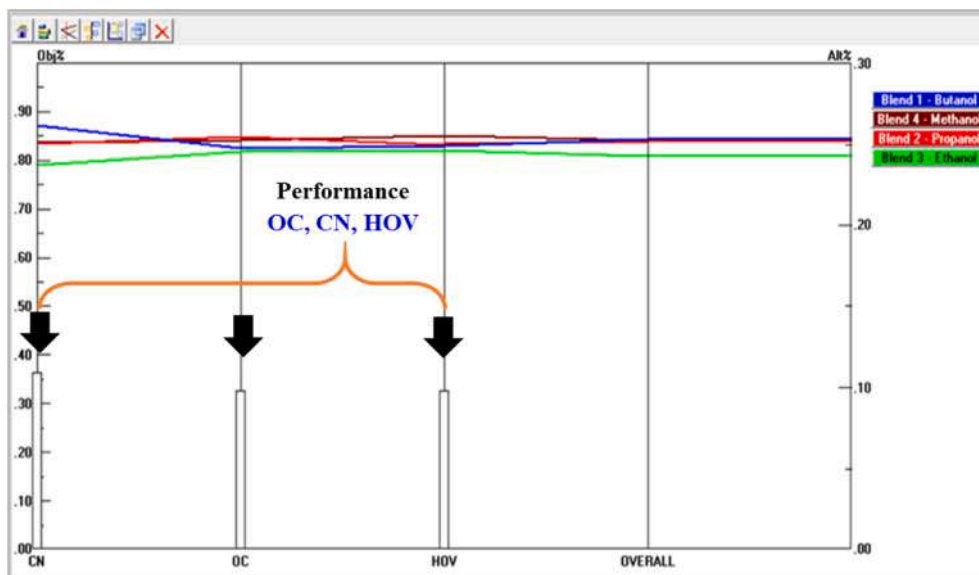


Fig. 13. Performance sensitivity graph of performance concerning goal when the priority vector of performance is increased by 20%.

Sensitivity analysis results are summarised in Table 7. Blend 1 (diesel/biodiesel/butanol) was concluded as the optimal clean diesel blend. In general, it can be observed that the performance sensitivity graph in Figs. 12-15 does not change when the four criteria weighting factor is increased up to 20% change. Significantly, the integrated product design indicated the most cost-effective and environmentally friendly clean diesel should contain 70% diesel, 20% biodiesel, and 10% butanol resulting in the highest CN, 48.69, with the lowest cost 1.2 USD/L and cleaner emission with 35% less sulphur concentration and 36% CO₂ emissions reduced (see Table 8).

4.3. Two-dimensional AHP-Sensitivity analysis

The two-dimensional sensitivity analysis demonstrates the priorities of the alternative concerning two objectives at a time (x-axis and y-axis). The area of the 2D plot is divided into quadrants. The most favourable alternatives concerning the objectives on the two axes are marked in the upper right quadrant. The closer to the upper right corner, the better the alternative. Fig. 16 points that Blend 1 has the lowest cost and the higher performance. The lowest cost for the alternatives shows the top correlation line as the blue dot for Blend 1 in the graphical sensitivity

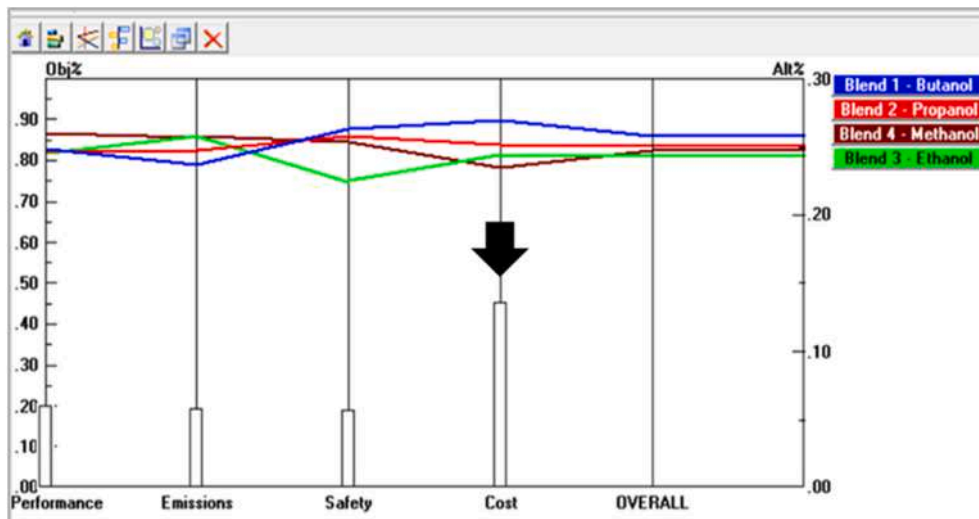


Fig. 14. Performance sensitivity graph of cost (USD/L) concerning goal when the priority vector of economic is increased by 20%.

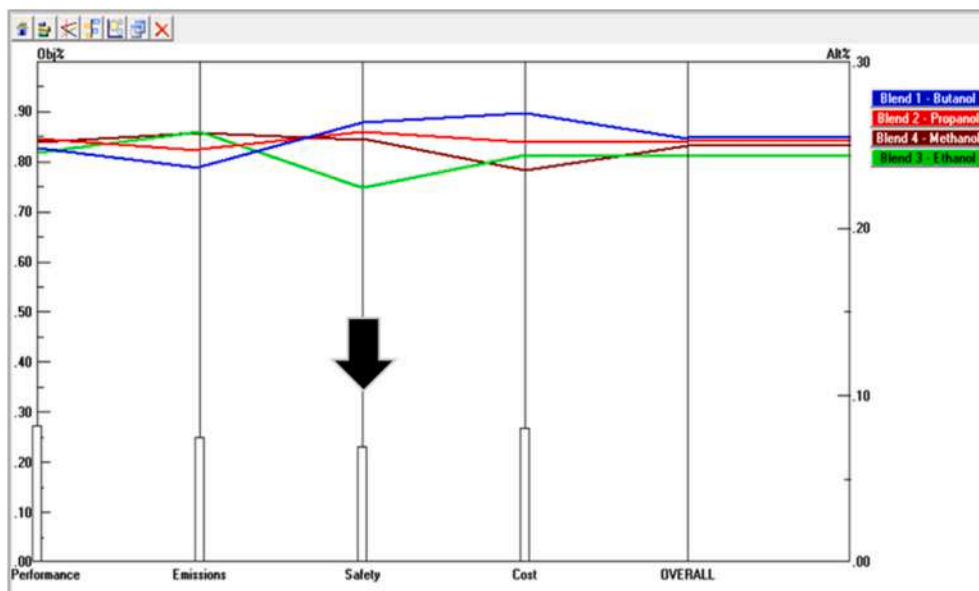


Fig. 15. Performance sensitivity graph safety concerning goal when the priority vector of economic is increased by 20%.

Table 7
The fuel properties of clean diesel blends.

Properties	Diesel/Biodiesel/Alcohol			
	Blend 1	Blend 2	Blend 3	Blend 4
Alcohol Used	Butanol	Propanol	Ethanol	Methanol
Diesel, x_D	0.70	0.65	0.67	0.70
Biodiesel, x_B	0.2	0.2	0.2	0.2
Alcohol, x_A	0.10	0.15	0.13	0.10
Density (kg/m ³)	843.15	842.84	838.45	840.65
Kinematic Viscosity at 40 °C (mm ² /s)	3.21	3.2	3.03	3.04
Cetane Number, CN	48.69	46.305	46.539	47.49
Calorific Value, CV (MJ/kg)	43.8	43.2	41.67	41.59
Heat of Vaporisation, HOV (kJ/kg)	465.12	412.81	365.95	441.51
Flash Point, FP (°C)	90.45	86.675	87.015	88.15
Oxygen Content, OC (mg/kg)	4.36	6.19	6.72	7.19
Sulphur Content (mg/kg)	0.17	0.19	0.17	0.18
CO ₂ emission (kg CO ₂ /L)	1.7283	1.8611	1.6689	1.7778
Cost, USD/L	1.2	2.9	2.6	1.7

analysis.

Blend 1 performs better and emits the lowest emissions with higher performance, as shown in Fig. 17. This analysis elucidated that Blend 1 is the optimal ternary clean diesel blends for all four scenarios evaluated, further validating the results gained through the pairwise comparison in the AHP method and the objectives (priorities) been computed.

The CN of Blend 1 is 48.69 approaching the CN of diesel (CN = 49), and is the highest CN among the four fuel blends (alternatives). The highest CN advantageously concludes that butanol has physical properties close to diesel fuels. Compared to lower alcohol, 10% of butanol exhibits better results even in lower blending concentrations. Also, the higher CN of Blend 1 concluded that only a minimal 10% volume of butanol is needed in attributing more powerful engine performance and improving the combustion efficiency and cleaner emissions simultaneously (Imtenan et al., 2015).

The higher CN associated with, the higher heat of vaporisation (HOV) of butanol than the lower alcohol promotes better fuel ignition and causes more air/fuel accumulations lowered cylinder pressure (Nanthagopal et al., 2018). This advantage of higher alcohol, such as

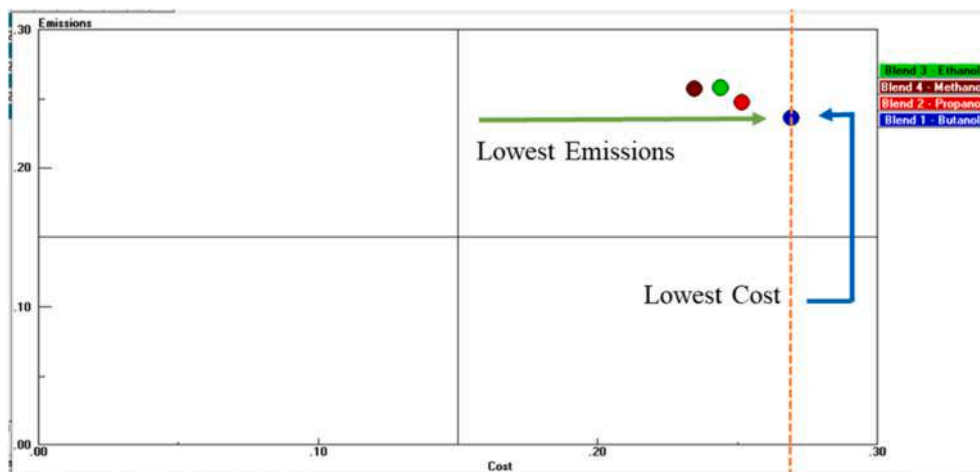


Fig. 18. Two-dimensional sensitivity of trade-off between cost and emissions.

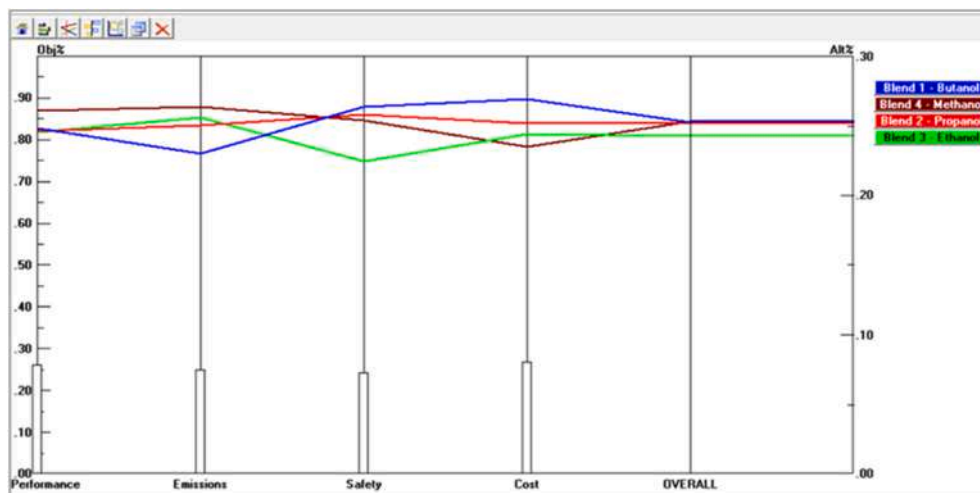


Fig. 19. Final synthesis with respect to the goal.

Blend 3 (diesel/biodiesel/ethanol).

Based on the rank chart of the sensitivity analysis summarised in Fig. 20, Blend 1 (diesel/biodiesel/butanol) ranked at the top for all four scenarios; economic, performance, cost, and safety. It is concluded that Blend 1 is the optimal ternary clean diesel blend. The final two-stage optimisation model significantly indicates the most cost-effective and

environmentally friendly diesel/biodiesel/butanol ternary clean diesel blends should contain 70% diesel, 20% biodiesel, and 10% butanol resulting in the highest CN = 48.69, with the lowest cost of 1.2 USD/L.

4.5. Tornado chart for sensitivity analysis

A tornado chart is a powerful visualization of the conclusion in making a decision. The tornado chart is a highly effective tool for illustrating sensitivity and risk management analyses. The tornado in sensitivity analysis provides a graphical representation of how the result is sensitive to the specified criteria.

The tornado chart in Fig. 21 demonstrates sensitivity analysis about the four different criteria; fuel performance (CN), emissions (OC and CO₂), cost, and safety (Flash Point). The larger bar shows that the safety factor is the most sensitive criteria and has the highest uncertainties in impacting the result. The cost variable listed at the bottom is the least important in affecting the objective.

Flash point (FP) is a significant parameter for safety measures in fuel blending. The FP of alcohols (FP = 12 °C–35 °C) is 50%–70% lower than diesel (FP = 72 °C). A liquid fuel with a lower flash point between 23 °C and 60 °C is considered a higher flammable, combustible, volatile, and hazardous liquid (Santos et al., 2020). For safety purposes, minimal alcohol oxygenates must blend with diesel/biodiesel to gain the same power output as diesel fuel.

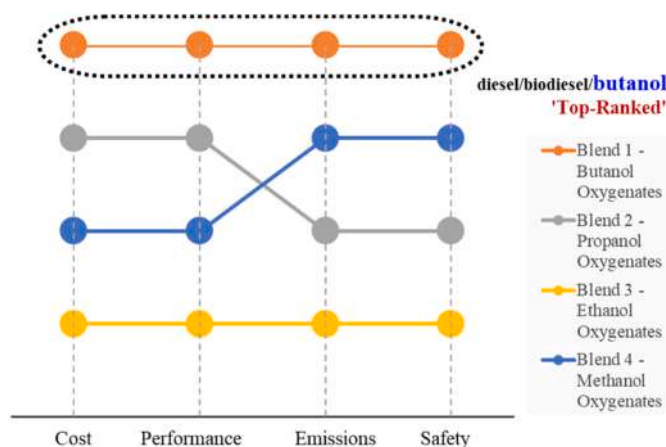


Fig. 20. The rank of alternative priorities for four alcohol oxygenates.

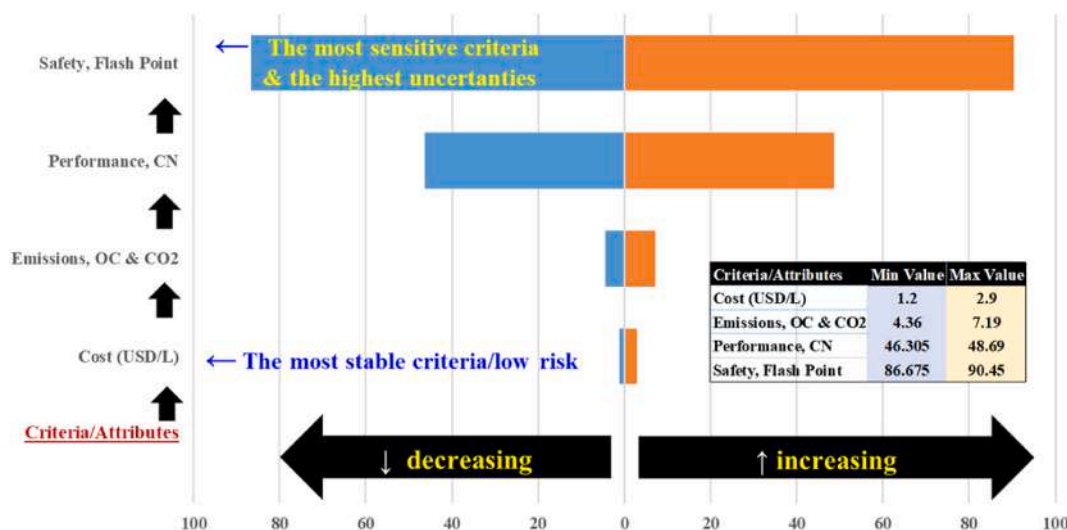


Fig. 21. Tornado chart for criteria (performance, cost, emissions, and safety).

This work identifies that 10% butanol in diesel/biodiesel blend increases the FP up to 90.45 °C, about 20% higher than FP diesel at 71 °C. The higher the flash point, the safer the fuel is regarding storage, transport, and handling. Higher alcohols (butanol) are preferably blended with diesel/biodiesel due to high FP over lower alcohols (Arnaldo et al., 2019). The higher FP of biodiesel at 184.5 °C makes the diesel/biodiesel/alcohol blends relatively stable for voluminous storage and safer handling.

Regarding the environmental impacts, the lower FP of alcohol advantageously reduces the fuel blend's viscosity and volumetric density simultaneously. With biodiesel's higher volumetric density and viscosity, a longer ignition delay will increase the peak pressure during the premixed combustion phase due to poor atomisation and spray characteristics (Pandey et al., 2012). The combustion temperature increased, which in turn increased the NO_x formation. The lower FP and higher volatility of alcohol reduce the compression work and combustion temperature due to higher HOV (Razak et al., 2021). The cooling effect of HOV leads to a lower combustion temperature and a reduction of NO_x emissions significantly.

4.6. Product analysis

Oxygenates with higher molecular weight (higher alcohol) such as butanol often have higher density, higher boiling point, higher viscosity, lower volatility, better lubricity, and lower flammability than respective oxygenates with lower molecular weight (lower alcohol) as ethanol (Imdadul et al., 2016). Consequently, oxygenates with higher molecular weight like butanol are preferred for diesel/biodiesel fuel blends components.

Butanol is the best oxygenate for CI diesel engines and provides several advantages over the lower alcohols; methanol, ethanol, and propanol. Ethanol precipitate dual-phase separation in diesel/biodiesel blends under 10 °C. Ethanol is not miscible with diesel at higher blend ratios because of low CN, leading to ignition delay due to its low calorific value and poor lubricity (Ali et al., 2015). With having good solvent capabilities, miscibility, and stability, butanol can be more easily blended with diesel/biodiesel without any engine modification.

Rajesh Kumar and Saravanan (2016) inferred that butanol has a higher miscibility factor due to its hydrophobic nature provides good solubility with diesel without phase separation. Butanol is less corrosive and can be stored in standard tanks for a longer duration (Chen et al., 2013). Moreover, the higher flash point of butanol (FP = 35 °C) than ethanol (FP = 17 °C) guarantees safe transportation, safe handling, and safe storage.

The advantages of butanol include higher CN and CV, which can reduce ignition delay, higher heat of vaporisation (HOV), and higher oxygen content (OC) that enables lower temperature in the cylinder and may improve the premixed combustion phase, leading to leading to a higher temperature to PM, CO₂ and NO_x emissions reduction. Significantly, butanol exhibits lower viscosity, which may cause better fuel atomisation, leading to complete combustion (Nanthagopal et al., 2018).

The interest in higher alcohol, such as butanol, has invigorated many CO₂ abatement initiatives due to its superior properties to methanol, ethanol, and propanol. Compared to the lower alcohols, the physico-chemical properties of higher alcohol are found to improve significantly and compensate for diesel/biodiesel blends while obtaining better results even in lower ratio blending concentrations (Mirhashemi and Sadrnia, 2020).

The butterfly diagram portrayed in Fig. 22 compares the relative importance of four variables: performance (CN), emission represented by oxygen content (OC) and CO₂ emissions, cost, and safety (flash point). The blue segments of the bars correspond to result in values for higher alcohol oxygenate, Butanol, and the orange segments of the bars correspond to results of lower alcohol, Ethanol.

The larger bars present the preferred (butanol) selection than the small bars (ethanol). This diagram means that uncertainty in performance, safety, emissions, and cost significantly impacts alcohol oxygenate selection, especially when comparing the lower and higher alcohol. Butanol 10% is the best candidate with higher performance, CN = 48.69, and lower cost at 1.2 USD/L.

Butanol is the best oxygenate for CI diesel engines and provides several advantages over the lower alcohols; methanol, ethanol, and propanol. The advantages of butanol include higher CN and CV, whereas can reduce ignition delay, lower heat of vaporisation (HOV) that enables higher temperature in the cylinder, and improve the premixed combustion phase, leading to NO_x emissions reduction.

In this study, the effect of four alcohol oxygenates (methanol, ethanol, propanol, and butanol) was investigated with various composition ratios on the combustion and emission characteristics in the diesel engines. This study focused on fuel properties enhancement. The effects of oxygen contents (OC), cetane number (CN), and heat of vaporisation (HOV) on exhaust emissions have been investigated systematically using model-based design optimisation.

The results show that higher alcohol (butanol) addition to diesel/biodiesel reduces 35% sulphur and 36% CO₂. The optimal Blend 1 comprises 70% diesel, 20% biodiesel, and 10% Butanol, indicating the highest performance (CN) associated and safer liquid (FP) with lower

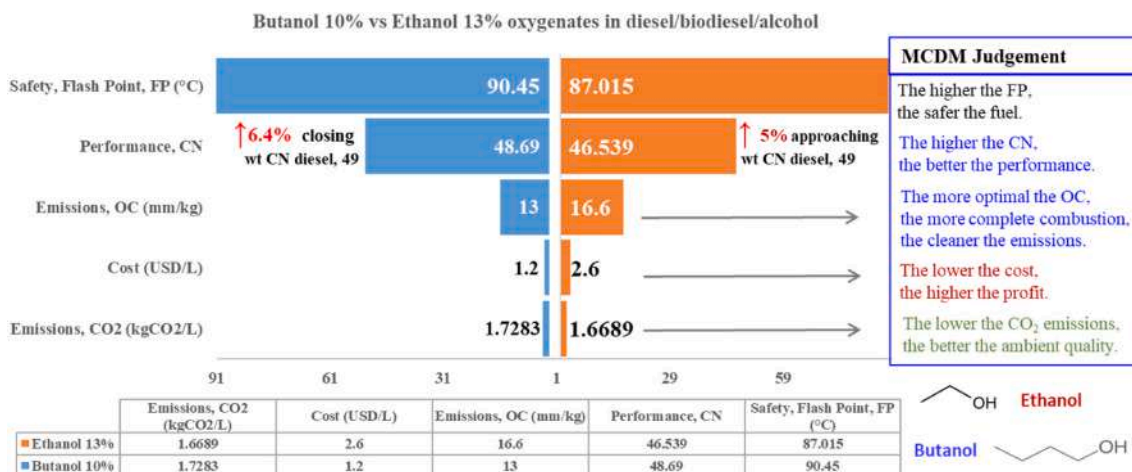


Fig. 22. Comparison results of butanol vs. ethanol with respect to criteria.

cost and lower emissions.

The effect of higher alcohol oxygenates, in particular, butanol, on performance (governed by CN), combustion characteristics, and environmental impact (governed by OC and HOV) have been reviewed. The following sub-conclusions are drawn as below:

- i. Fuel properties such as CN, OC, and HOV of alcohols oxygenate significantly reduce the diesel exhaust emissions.
- ii. Higher alcohol (butanol) offer superior characteristics such as higher OC (promotes complete combustion to reduce sulphur, PM, CO₂, smoke, and soot), higher HOV (stronger cooling effect to reduce NO_x), CV (higher power output), CN (reduces ignition delay), density and viscosity (better fuel flow for better atomisation), and flash point (for safer storage and handling), as compared to lower alcohol like ethanol.
- iii. A two-stage model-based fuel blends design optimisation that integrated LP and AHP is the best strategy in predicting, designing, and executing experimental investigation of fuel blends on engine performance, exhaust pollutants, safety systems, and combustion characteristics.

5. Conclusions

This paper presents a new and systematic two-stage model-based fuel blends optimisation that integrates linear programming (LP) with AHP to select the best alcohol oxygenates for diesel/biodiesel/alcohol fuel blends. This integrated model has adopted a hybrid MCDM method, MODM, and MADM to evaluate the trade-offs such as quality and quantity merits. Four criteria have been evaluated, including performance, emissions, cost, and safety, which are significant in the complex fuel blending optimisation model.

The final result depicts 70% diesel, 20% biodiesel, 10% butanol as the optimal diesel/biodiesel/alcohol fuel blends at the higher performance (CN = 48.69 ≈ CN Diesel = 49), safer handling fuel (higher flash point), and fewer environmental impacts at minimal cost (1.2 USD/L). The higher cetane number (CN) and oxygen content (OC) and heat of vaporisation (HOC) of butanol oxygenates in diesel/biodiesel promote cleaner diesel emissions with 35% less sulphur concentration and 36% CO₂ emissions reduced.

This two-stage fuel blends optimisation model, consisting of quantitative (MODM) and qualitative (MADM) merits, prohibit the robustness of this novel fuel blending optimisation model, to get the best optimal result that fulfills the three sustainability models; (economic, social and environmental) plus product safety.

Compared to the conventional optimisation algorithm, this two-stage fuel blends optimisation model provides the confident decision to select

alcohol oxygenates for diesel/biodiesel/alcohol without an extensive experiment, thereby saving time and money and reducing harmful environmental impacts.

5.1. Technical limitations

Despite the significant benefits inherent in mathematical optimisation in product design, there are also substantial challenges and limitations regarding this process and the continuous conduct of the strategy. This study has three primary limitations to the generalization of these results that could be addressed in future research as below:

i. Constraint Parameters

The design objective is limited by blends, product property, and process model constraints. Any factors that proscribe the formulation of blends are called blends constraints. An example of blends constraints is the miscibility/solubility property that indicates the phase behaviour of the blends. The miscibility is very important in liquid blending because it determines the feasibility of the optimal blends (Agarwal, 2007; Yunus and Manan, 2016). A property constraint model represents the target properties defined from the product needs, such as type of fuel blends, volume fraction, and blends miscibility. The product property constraint is unique for each product design problem. The process model constraint denotes the conditions for the blending process, for example, mass balance. A restriction on the design parameters is also considered a process model constraint, such as the limitation of the composition in blends. Blends formulation should be considering multiple types of constraint equations to get the feasible and optimal blends.

ii. Multiple objective functions

The product design typically deals with optimisation with respect to one objective. Since business-industrial requirements are not fully satisfied with only one objective, generally by quantitative merits. In fuel blending, qualitative factors must also be considered when making the final decision. It is necessary to consider several even competing objectives.

The performance of clean diesel is evaluated from the blends' cetane number (CN). Besides enhancing the fuel performance, the new formulation of clean diesel blends (diesel/biodiesel/alcohol) should be safe, cost economics, and have low environmental impacts.

Fuel blending is often challenging because they contain an overwhelming boundary of design trade-offs such as quality and quantity merits of fuel performance, safety strategy, cost-effectiveness, and environmental issues. The LP model only evaluates solutions concerning

quantitative criteria with one single objective function. In fuel blending, qualitative factors must also be considered when making the final decision. As a result, the fuel blending optimisation problem should rely extensively on hybrid MCDM methods, quantitative (MODM), and qualitative (MADM) approaches.

iii. Sample size and model reliability

Another limitation is the model reliability, where solving the blending problem using a mathematical approach requires property models that are predictive and accurate. Sample sizes can also become a huge problem and increase exponentially with the size of the database and type of the blends. The size of the problem depends on the number of fuels used for blending and the type of blends. If it is impossible to find a large enough sample size, the data collected may be insufficient. Solving a complex optimisation problem mathematically requires extensive computational efforts and may cause non convergence and more collapse results.

5.2. Research implications

An integrated two-stage optimisation has resulted from this study, which is very helpful for the policymakers, industrial players, and researchers to generate interdisciplinary perspectives to inform policies and development at a national level, especially from a low-carbon pathway context. It is essential to address this initiative to inform energy systems planners and policymakers when deciding whether to focus on pursuing new biofuels blended with diesel with cleaner emissions at a minimal cost.

In addition, focus on strengthening current policies that promote dedicated biomass technologies and other renewables. This insight is important because, in several developing countries, policies promoting biofuels such as oxygenate alcohol remain unavailable, although policies promoting renewables are already incorporated in national policies. In this way, if a conflict arises between the policy goals, decision support tools can inform policymakers on the synchronization of those multiple policies.

Aside from providing an incentive to the bioenergy producers, these systematic two-stages optimisation models for the clean diesel blends could be potentially brought down in the future through technological learning. This aspect is related to the minimization of the investment cost of technologies. Technological learning can make the most progress in Malaysian biofuels, for example, biodiesel and bioalcohol as oxygenates based on learning from foreign technology partners and internal knowledge by planned experimentation.

5.3. Recommendations for future works

The following recommendations are listed to address the issues related to this research work:

The two-stage fuel blends optimisation model concurrent Linear Programming (MCDO) and AHP (MCDA) provides the confident decision to select alcohol oxygenates for diesel/biodiesel/alcohol without an extensive experiment, thereby saving time and money and reducing harmful environmental impacts.

Using the results of this paper as an objective function in a biofuel formulation design model can be useful. The proposed framework can also be used for other liquid biofuels, like biodiesel, esters, biomass-based biofuels from crops such as corn cob, sugar cane, and different base fuel such as gasoline and kerosene future research can examine.

Technology selection for biomass to biofuels conversion process is also important to recognize all the variables/characteristics. This opens up a new path for researchers to further study and decide the best conversion technology for biorefinery production.

CRedit authorship contribution statement

Nurul Hanim Razak: Investigation, Methodology, Software, Writing – original draft, Visualization. **Haslenda Hashim:** Conceptualization, Methodology, Validation. **Nor Alafiza Yunus:** Data curation, Formal analysis. **Jirí Jaromír Klemes:** Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing for financial interests or personal relationships that could have influenced the work reported in this paper.

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