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Quantifying the effects of fuel compositions on GDI-derived particle emissions using the optimal mixture design of experiments

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HIGHLIGHTS

- Mixture design DoE can be used to construct Particle Number (PN) models.
- Aromatics produced more PN emissions for nucleation and accumulation mode PM.
- The ANOVA shows that the derived PN model is statistically significant.

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ABSTRACT

The relationship between fuel compositions and particulate matter (PM) emissions originating from a gasoline direct injection (GDI) engine was explored and used to identify optimal fuel composition for minimizing the number concentrations of both nucleation mode and accumulation mode PM via a predictive PM model developed by using optimum mixture design DoE (Design of Experiments). N-octane, isooctane, xylene and ethanol, were blended to form test fuels according to the DoE design, and the solid Particle Number (PN) emissions were measured by a particle spectrometer DMS500. The responses for the DoE design were the nucleation mode PN and accumulation mode PN. The results indicated that aromatics produced more PN emissions, whilst the effects of other fuel components on the PN emissions were unclear because of the interactive effect arising from different combinations of fuel substances. Two non-linear mathematic models for both modes PN were validated experimentally according to ANOVA analysis.

1. Introduction

As particulate matter emissions are highly correlative with the properties of fuels [1–4], it is possible to predict particle emissions from the physical and chemical properties of fuel substances. Several studies have successfully derived either PM (Particle mass) or PN (Particle Number) regression models to quantify the effects of different factors on the PM emissions [5–7]. Regarding fuel properties related models, Honda Motor Company Ltd. [6] proposed a predictive model for PFI engines, termed as the 'PM Index', based on the weight fraction, vapor pressure, and DBE value of each component in the fuel. Researchers found that components with a high boiling point, low vapor pressure and a high double bond equivalent (DBE) value tend to produce more particulate number (PN) emissions. The PM emissions predicted by this model fitted the experimental values consistently. A good correlation between fuel PM Index and PM emissions was achieved for a range of PFI engines burning various fuels.

Nevertheless, there has been no independent control of vapor pressure and the DBE value when commercial fuels were used and insufficient fuel compositional information that would inhibit the calculation of the PM index. In order to solve these problems and improve the accuracy of the prediction of PN emission, Oxford incorporated modified Raoult's law into the existing PM index model. A new PN index was formulated and the predicted results fit the GDI engine experiment results adequately [7]. This model can be used to ensure co-evaporation of aromatic and paraffin components in a model fuel, to avoid stratification of the individual components of a fuel in-cylinder. The PN index has been validated in a GDI engine by using both model fuels and commercially available fuels.

Both the Honda PM index and the Oxford PN index correlated the PM emissions to the fuel physical and chemical properties with DBE reflecting the fuel chemical characteristics. However, this value is an ensemble property of the whole fuel as a mixture and

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Nomenclature

ANOVA	Analysis of Variance
CPMA	Centrifugal Particle Mass Analyzer
DBE	Double Bond Equivalent
ECU	Electronic Control Unit
DoE	Design of Experiment
DVPE	Dry Vapor Pressure Equivalent
EGR	Exhaust Gas Recirculation
GDI	Gasoline Direct Injection
MBT	Minimum Best Torque
PDF	Probability Density Function
PM	Particulate Matter
Pm	Particle Mass
PN	Particle Number
RON	Research Octane Number
SGDI	Spray Guided Direct Injection
TWC	Three-Way Catalyst

it lacks detailed information on individual fuel component. In addition, the physical properties may well be reliant on chemical compositions. Given the above considerations, an attempt was made to establish a quadratic model linking individual fuel components and the PM emissions.

In order to construct the model in a more systematic manner, a mixture design approach was adopted to explore the individual effects and the associated interactions of fuel components in a mixture on the PM emissions. The mixture design approach is a unique type of DoE (Design of Experiment) technique which provides an efficient means of optimizing the processes as well as determining the optimal formulation of a specific mixture [8]. The primary reason to select mixture design DoE as compared to other types of DoE is that the sum of the input variables, in this case individual fuel components, must be unity. This allows a restriction on the ranges of component fractions to thus fit the mathematical models for predicting PM tendency of fuel. Furthermore, the measured responses are particle number concentrations for nucleation mode and accumulation mode which are assumed to depend only on the relative proportions of the fuel ingredients rather than the absolute quantity of each component.

Two software packages, namely, Design Expert and Minitab, were used in parallel to accomplish the mixture design DoE. Both gave effectively the same results and the predicted models fit the experimental data with a statistically higher significance as demonstrated in the following ANOVA (Analysis of Variance) discussion. This work demonstrated that the mixture design DoE is a useful tool to quantify the effect of fuel compositions on PM emissions by constructing PM or PN index models. However, the models proposed herein are not universally applicable as the results are bound to be subject to changes in other parameters such as engine operating conditions.

2. Material and methods

2.1. Fuel formulation and mixture design DoE

The primary characteristic of mixture design DoE is that the input variables or components are non-negative proportionate amounts of the mixture. If the relationship is expressed as fractions of the mixture, the sum must be equal to unity. Furthermore, in mixture design DoE, the measured response is assumed to depend only on the relative proportions of the ingredients or components in the mixture and not on the volume of the mixture [9,10].

In most mixture designs, the upper and lower limits imposed on each component proportion X_i, which are termed as a_i (lower limit) and b_i (upper limit). The general form of the constrained mixture problem is given as:

$$0 \leqslant a_i \leqslant X_i \leqslant b_i \leqslant 1 \text{ and } \sum_{i=1}^{n} X_i = 1 \quad (1)$$

where $i = 1, 2, 3, \ldots, n$.

And the response Y is expressed as a function of the independent factors X_i:

$$Y = f(X_1, X_2, X_3, \ldots\ldots X_n) \quad (2)$$

A typical mixture design DoE involves the following steps [8]:

1. Select a suitable technique of mixture DOE based on the ranges of the independent variables or bound restrictions.
2. Identify the name, unit and the bound restrictions of mixture components;
3. Identify the name and unit of the responses.
4. Propose an appropriate model to find the relationship between the responses and the mixture components.
5. Run all the determined experiments designed by the model in consecutive order as accorded to the run numbers.
6. Enter the achieved responses from the experimental results.

Four groups of compounds, n-alkane, iso-alkane, aromatic and alcohol were used to formulate the test fuels. N-octane, isooctane, xylene and ethanol were chosen to represent the aforementioned four chemical groups. To ensure the stability of engine operation, the fraction of each compound was designed so that the total RON (Research Octane Number) value was approximately between 90 and 100. Given the fact that the market share of alcohol in transportation consistently increased and the dramatic impact on PM emissions, the range of ethanol fraction was chosen to be 10–25%, whilst the fractions of the other 3 groups were 5–10%, 40–60%, and 25–35% for n-octane, isooctane and xylene, respectively, which is in accordance with the national standard (GB 17930-2011 [11]) The physical and chemical properties of the four fuel substance used are listed in Table 1.

Based on the Extreme Vertices Design Theory [12,13], nine combinations of test fuels are determined as shown in Table 2, where 1 represents vertex and 0 represents barycenter for point type.

Nine blends were prepared according to Table 2 proposed by the mixture design DoE algorithm. It can be noted that the slight difference in the densities needs be taken into account to convert mass fractions to volume fractions for convenience when mixing the test fuels. The center point, in this case fuel 7, was replicated

Table 1
Physical and chemical properties of the four fuel substance.

Name	N-octane	Isooctane	Xylene	Ethanol
Mass fraction	5–10%	40–60%	25–35%	10–25%
Chemical formula	C_8H_{18}	C_8H_{18}	C_8H_{10}	C_2H_6O
H/C ratio	2.25	2.25	1.25	3
Density (kg/L at 20 °C)	0.70	0.6919	0.86	0.80
RON	−10	100	117	114
Boiling point (°C)	126	99	138	79
Auto-ignition temperature (°C)	220	417	528	363
Flash point (°C)	13	4.5	27	13