

CRC Report No. RW-107-2

An Improved Index for Particulate Matter Emissions (PME)

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CRC Project No. RW-107-2:

An Improved Index for Particulate Matter Emissions (PME)

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COORDINATING RESEARCH COUNCIL

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CRC PROJECT NO. RW-107-2:

Emerging PMI Methodologies

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LIST OF ACRONYMS

AKI	Anti Knock Index
ASTM	American Society for Testing and Materials
CO	Carbon Monoxide
CO ₂	Carbon Dioxide
CRC.....	Coordinating Research Council
DBE.....	Double Bond Equivalent
DHA.....	Detailed Hydrocarbon Analysis
DOE	U.S. Department of Energy
EPA.....	U.S. Environmental Protection Agency
E0	Fuels that do not contain ethanol
E10	Fuels containing 10 vol% ethanol
E15	Fuels containing 15 vol% ethanol
E20	Fuels containing 20 vol% ethanol
E>0.....	Fuels containing ethanol at any level
EtOH	Ethanol Content
FID	Flame Ionization Detector
GC	Gas Chromatograph or Chromatography
GHG.....	Greenhouse Gas
MAE	Maximum Absolute Error
MS.....	Mass Spectrograph or Spectroscopy
MSD.....	Mass Selective Detector (in GC)
MW	Molecular Weight
NMHC.....	Non-Methane Hydrocarbons
NMOG	Non-Methane Organic Gases
NO _x	Oxides of Nitrogen
PASCE	Particulate and Soot Correlation Equation
PEI.....	Particulate Evaluation Index
PIONA	Hydrocarbon Speciation using ASTM D8071
PM.....	Particulate Matter
PME-A	PME Index (ASTM DHA)
PME-B	PME Index (AVFL-29 DHA)
PMI	Particulate Matter Index (ASTM DHA)
PMI-A	Particulate Matter Index (AVFL-29 DHA)
PN	Particle Number
PFI.....	Port Fuel Injection
R ²	Coefficient of Determination
RMS	Root Mean Square
RVP.....	Reid Vapor Pressure
SIDI.....	Spark-Ignited Direct-Injection
SSI.....	Separation Systems, Inc.
SwRI	Southwest Research Institute
THC.....	Total Hydrocarbon
US	United States
VP _{443K}	Vapor Pressure at 443K
YSI	Yield Sooting Index

EXECUTIVE SUMMARY

Over the past 10 years, significant research work has been undertaken to quantify particulate matter (PM) emissions from gasoline vehicles and to investigate their relationship to fuel properties and composition. In prior research on this topic by CRC, EPA, and others, the Honda Particulate Matter Index (PMI) was used as a measure of a gasoline's potential to cause PM emissions from vehicles.

In CRC Project RW-107, the Honda PMI and several simplified, correlation-based PM and soot indices were evaluated to determine their efficacy in predicting LA92 Phase I¹ PM emissions based on fuel composition and properties. PMI was found to perform well *if* the fuels being evaluated had the same ethanol content, but it proved to be a biased indicator when applied to groups of fuels with varying ethanol content – i.e., E0 (neat), E10 (10% ethanol by volume), and higher ethanol-content fuels. LA92 Phase I PM emissions from fuels with ethanol were found to be consistently greater than emissions from non-oxygenated fuels of the same PMI.

To fill the need for a metric capable of indicating PM emissions potential for a broad range of fuels, including oxygenated fuels, CRC initiated Project RW-107-2 to examine alternative mathematical formulations to PMI. The objectives were to eliminate the Honda PMI's ethanol bias and to create a “new technology” PM index that could inform fuel research and blending of in-use fuels into the future.

The work in this project examined a series of alternate mathematical formulations of PMI until one was found that captured all major elements of PM formation in gasoline engines. The resulting index—known as PME—is linearly correlated with Phase I PM emissions over the LA92 driving cycle in vehicles powered by spark-ignition direct injection (SIDI) and port-fuel injection (PFI) engines. The acronym PME (Particulate Matter Emissions) was chosen to indicate that it was developed to be linear with LA92 Phase I PM *Emissions* and distinguish it from the Honda PMI. It is applicable to both non-oxygenated and oxygenated fuels containing different functional groups and quantities of oxygenated compounds. Like the Honda PMI, PME relies on speciation of the fuel using a Detailed Hydrocarbon Analysis (DHA) based on ASTM procedures or an alternative procedure developed by Separation Systems, Inc. (SSI) under CRC Project AVFL-29.

The improvements of PME over PMI account for:

- An improved, empirically based measure of each hydrocarbon compound's chemical propensity to form soot, including oxygenated compounds used in fuels;

¹ The cold-start phase during which the largest share of PM is emitted in both SIDI and PFI engines.

- The enrichment of fuel droplets, or localized areas with rich air-fuel ratios, in heavy hydrocarbons (compared to the overall composition of the fuel) because of the faster vaporization of lighter compounds as the fuel charge heats;
- How the presence of ethanol in a fuel accelerates early vaporization and cools the fuel charge, leading to further enrichment of fuel droplets and localized areas with rich air-fuel ratios; and
- How changes in the energy density of fuels influence the quantity of fuel needed to propel a vehicle and, thus, its PM emissions in terms of the PM mass emitted per unit distance.

Table ES-1 provides the PME formulation along with the coefficients appropriate for use based on fuel system technology (either PFI or SIDI) and DHA type (either ASTM or SSI). The index is written as PME-A when evaluated using an ASTM DHA and as PME-B when evaluated using an SSI DHA. Here, “ASTM” is a generic label that covers different versions of the DHA method (including D6729, D6730, and D6733), but it is typified by ASTM D6730 as practiced in research laboratories during the period 2016-2018. The $yTerm_i$ parameter gives the chemical sooting propensity of each compound in the fuel based on the number of carbon and oxygen atoms (molecule “size”), counts of the double bond equivalents (DBEs) found outside of aromatic rings, and the count of aromatic rings, if any.

Table ES-1
The PME Formulation

$PME = \left(\frac{43.4}{LHV} \right) \cdot [N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}]^\beta$ $\alpha = \{ \alpha_{E0}, \alpha_{E10}, \alpha_{E20} \}$ $f(EtOH) = \alpha_{E0} + \Delta\alpha \cdot EtOH_{VOL\%}$ $LHV = \text{Lower Heating Value}$							
$yTerm_i = (C+O-1) \cdot (1 + 1.7 \cdot DBE_{NON} + 5.6 \cdot ArRing_{FIRST} + 5.1 \cdot ArRings_{ADD})$							
Engine Technology	DHA Type	Designation	N _{TECH}	α _{E0}	α _{E10}	α _{E20}	β
SIDI	ASTM	PME-A	0.00597	0.456	0.443	—	1.17
	SSI	PME-B	0.00597	0.456	0.443	—	1.00
PFI	ASTM	PME-A	0.0109	0.564	0.558	0.531	1.17
	SSI	PME-B	No data is presently available				
Note: Green font denotes empirically estimated parameters.							

PME’s performance was evaluated using the datasets on which it was based: CRC E-94-2 for SIDI vehicles and EPAAct for PFI vehicles. The evaluation showed that PME is linearly proportional to LA92 Phase I PM emissions on the fuels and without bias with respect to ethanol content. Given the data utilized, the performance of PME has been demonstrated

for fuels having Reid Vapor Pressure (RVP) values of ~7 psi for SIDI vehicles and 7~10 psi for PFI vehicles.

However, PME *should not* be used to guide the addition of ethanol to a blendstock for oxygenate blending (BOB) to create a finished fuel. PME does not accurately indicate the PM potential of the BOB itself. But PME will indicate the PM potential of the resulting finished fuel in comparison to *other finished fuels of similar RVP*.

1. INTRODUCTION

1.1 Background and Objectives

Automotive engine technology has changed substantially in the past two to three decades under the influence of increasingly stringent tailpipe emissions and fuel economy standards in the United States (US) and other countries. Such pressures led early on to the replacement of carburetors with port fuel injection (PFI) systems to permit precise control of the air-fuel mixture. More recently, new engine technologies such as the Spark Ignition Direct Injection (SIDI) engine use sophisticated computer control and in-cylinder injectors to deliver atomized gasoline directly into the cylinder (rather than the intake manifold) in an effort to maximize engine output and minimize fuel consumption.

Combustion in gasoline engines can produce particulate matter (PM) in localized areas with rich air-fuel ratios or when heterogenous combustion involving liquid fuel droplets occurs. In SIDI engines, this occurs throughout all phases of driving, although the largest share of PM is emitted during cold start operation. In PFI engines, this occurs mainly during cold-start and is greatly diminished once the engine becomes fully warm.

With the introduction of SIDI technology, gasoline droplets injected into engine cylinders are combusted over a wide range of operating modes. Cold-start operation continues to be the phase when the most PM is emitted, but PM can be emitted even after engine warm-up. Recent research has shown that PM emissions from SIDI vehicles are generally higher than from PFI vehicles, although some SIDI designs have demonstrated comparable emissions (Saliba 2017). In addition to engine and emission control design, the composition and properties of gasoline fuels have been shown to influence PM emission levels in both engine types.

In research on the PM emissions of gasoline vehicles and the relationship to fuel composition and properties, the Particulate Matter Index (PMI) introduced by Honda has found widespread acceptance as a way to measure a gasoline composition's potential to contribute to PM emissions. The PMI is based on a profile of the individual hydrocarbons in a fuel as determined through a Detailed Hydrocarbon Analysis (DHA), typically using the ASTM D6730 procedure (as in the PMI's development). Data generated from variants of the ASTM DHA procedure also have been used to determine PMI for fuels.

Given a DHA, the PMI for a fuel is calculated using the Honda Equation:

$$\text{PMI} = \sum_i W t_i * \left(\frac{1 + DBE}{VP \text{ at } 443K} \right) \quad (3-1)$$

Here, DBE is the count of double-bond equivalents in each compound, including double-bonds and their equivalents in the form of triple bonds and rings. The numerator $1 + \text{DBE}$ was adopted as the indicator of a compound's propensity to soot based on the research available at the time (Aikawa 2010).

The Honda PMI and several simplified, correlation-based PM and soot indices were evaluated in CRC RW-107 to determine their performance in predicting the PM emissions potential of fuels. PMI was found to perform well *if* the fuels shared the same ethanol content, but it proved to be a biased indicator when applied to mixed groups of neat gasoline and ethanol-containing fuels. LA92 Phase I PM emissions from the ethanol-containing fuels were found to be consistently greater than emissions from the neat fuels of the same PMI.

To fill the need for a PM index that can indicate the PM emissions potential for a broad range of fuels, CRC initiated Project RW-107-2 to examine alternative mathematical formulations for a PM index. The objective was to eliminate the Honda PMI's ethanol bias and to create a "new technology" PM index that could serve fuel research and fuel blending into the future. The result of this work is the PME (Particulate Matter Emissions) index, so named to indicate that it is defined to be linear with LA92 Phase I PM Emissions. Phase I of the LA92 cycle is the cold-start phase during which the largest share of PM is emitted.

The development of PME evolved over the course of one year through examination of a series of different mathematical formulations, as if the layers of the PM index problem were peeled back one-by-one. This report does not attempt a step-by-step explanation of the development process but, rather, serves to document the end result in sufficient detail that potential users can understand the PME index, how to apply it, and the empirical underpinnings on which it is based.

1.2 Report Organization

The report is organized as follows. Section 2 gives a brief summary of the several datasets on which this work is based, including the vehicle emissions datasets used to estimate and evaluate PME; the Yield Sooting Index (YSI) dataset on the chemical sooting potential of hydrocarbons; and the two types of DHAs (ASTM² and SSI DHA³) used here to determine the hydrocarbon composition of the experimental fuels. Further information is available in the published reports for CRC RW-107 and for the individual emission studies previously mentioned.

Section 3 presents the empirical underpinnings of the PME formulation and how it represents the several elements of PM formation in vehicles. The objective is to explain to potential users what the individual terms in PME mean and how they were developed from

² ASTM DHAs are defined by ASTM standards including ASTM D6729, ASTM D6730, and ASTM D6733.

³ The SSI DHA was developed by Separation Systems Inc. (SSI, Gulf Breeze, FL) under CRC Project AVFL-29.

empirical data. The three subsequent sections present the PME index based on specific datasets, as follows:

- Section 4: SIDI vehicles using an SSI DHA.
- Section 5: SIDI vehicles using an ASTM DHA.
- Section 6: PFI vehicles using an ASTM DHA.

None of the datasets available to this study cover emissions from PFI vehicles on fuels for which a SSI DHA has been performed. Thus, it is not possible to propose a PME index for PFI vehicles and SSI DHAs at this time.

The PME index will be used primarily in fuel research, but not in fuel blending where simpler methods not involving a DHA are needed. Section 7 discusses the effort, ultimately unsuccessful, to update the simpler, correlation-based PM indices that were examined in CRC RW-107, the preceding project.

Finally, Section 8 provides a concluding discussion of the PME index and its applicability to real-world fuels. Caveats to its application are discussed as well as steps that CRC is taking to validate the PME index using new and independent datasets. Finally, the discussion covers how differences between PME and the Honda PMI may affect the conclusions of prior studies on the effect of ethanol blending on PM emissions. Section 9 lists the references cited here.

Three appendices have been prepared to document the data and analysis performed in this work:

- Appendix A contains a master list of information on hydrocarbons compounds that will be needed by potential users interested in evaluating PME for their fuels. It includes the counts of carbon and oxygen atoms and the bonds and rings by compound that are needed to evaluate the y_{Term} numerator of PME. It also includes updated and standardized data on boiling point (BP) and vapor pressure at 443K (VP_{443K}) that were used here and are recommended for use with PME.
- Appendix B explains the methodology for estimating the PME index from PM emissions datasets.
- Appendix C tabulates the PME-A and PME-B index values for each experimental fuel in the studies used in this work.

Supplementary material for this work is available from the CRC website, including the following:

- An Excel version of the master list of hydrocarbon compounds contained in Appendix A (CRC RW-107-2 AppA.xlsx).

- A PowerPoint presentation in pdf format (CRC RW107_2_DHAReference.pdf) that documents the DHA sources for the experimental fuels used here and the Honda PMI values that result from the update and standardization of inputs on BP and VP_{443K} for hydrocarbon compounds.

2. DATA USED IN THIS WORK

2.1 Vehicle Emissions Datasets

This section reviews the primary characteristics of the PM emissions datasets used in developing the PME formulation. The CRC E-94-2 study was the basis for developing the PME formulation for SIDI vehicles and estimating its coefficients; both ASTM and SSI DHAs were available for their fuels. The mathematical formulation of PME-A for SIDI vehicles was retained for PFI vehicles. The EPAct study was the basis for estimating the coefficients of PME-A for PFI vehicles. Only ASTM DHAs are available for its fuels as the EPAct study was done a decade before the SSI DHA method was developed.

A more extensive discussion of these two studies can be found in the published report for CRC RW-107, the predecessor study to the present one. Further information on the vehicles and fuels can also be found in the respective published reports for the emissions studies. References to the published reports can be found in Section 9 where they are identified by the study names (CRC RW-107, CRC E-94-2, and EPAct).

2.1.1 CRC E-94-2 Study

The CRC E-94-2 study investigated the particulate and gaseous emissions of a test fleet of 12 vehicles equipped with SIDI engines that were manufactured in model years 2010 through 2015. As a group, the vehicles were considered to be representative of the range of SIDI models available in the US at that time.

Eight different fuels were blended for the study according to a design matrix based on octane rating (AKI), ethanol content (EtOH), and Honda PMI level. Two AKI levels were targeted: 87 AKI, representative of regular grade gasoline; and 93 AKI, representative of premium grade in much of the US. Four fuels were blended within each octane level to fill a 2 x 2 matrix of ethanol content (E0 and E10) and PMI level (Low PMI ≤ 1.40 and High PMI ≥ 2.4). The characteristics of the fuels, as blended, are given in Table 2-1.

The overall objective was to create fuels that, to the extent possible, would be representative of commercial gasoline across the typical range of octane levels, ethanol contents, and PMI values. The measured properties of the resulting fuels were checked to assure that each fuel met the specifications for commercial gasoline. For this reason, the set of match-blended E-94-2 fuels is believed to be the most representative of US gasolines among the emissions studies used here. However, they are only eight in number and do not explore the full range in variation for fuel characteristics that may influence PM emissions.

Particulate and gaseous emissions of the vehicles were measured at the Southwest Research Institute (SwRI) laboratory in San Antonio, TX, using the LA92 test cycle. Emissions were reported for the individual phases of the cycle and as LA92 weighted-averages. Both particulate mass (PM) and particle number (PN) were measured along with subcomponents (elemental and organic carbons). Gaseous emissions were measured as well, including total hydrocarbons (THC), carbon monoxide (CO), nitrogen oxides (NO_x), and carbon dioxide (CO₂).

Table 2-1
Experimental Fuels used in E-94-2

Fuel	AKI	EtOH* vol%	PMI
A	87.2	9.55	1.42
B	87.1	9.56	2.65
C	87.9	0	1.40
D	88.2	0	2.61
E	93.6	9.56	1.28
F	93.7	9.51	2.54
G	93.8	0	1.26
H	94.1	0	2.49 [†]
* Based on ASTM D4815. [†] The PMI value for Fuel H has been corrected from that published to reflect the re-analysis of the retained sample at the start of the E-94-3 program. The revised value, determined by Lab C, is consistent with the PMI value also determined by Lab C for the splash-blended Fuel H-C10. The PMI values for the E-94-2 fuels published in Appendix A of the CRC E-94-2 Report (2017) are based on averages for three laboratories. Source: Table 3. CRC E-94-2 Report (2017).			

2.1.2 EPAAct Study

The EPAAct study—a joint research project involving EPA, the US Department of Energy (DOE), and CRC—was conducted in phases between 2007 and 2013 to understand how trends in vehicle technology since the 1990s had changed the relationship between vehicle emissions and gasoline properties. The present study uses the EPAAct Phase 3 emissions results, which are documented in three reports: EPAAct (2013a) Analysis of Data; EPAAct (2013b) Program Design and Data Collection; and EPAAct (2010) Fuel Blending.

EPAAct focused on five key characteristics of gasoline: aromatics and ethanol contents, RVP, and the T50 and T90 boiling points. Its test fleet of 15 vehicles from model year 2008 included passenger cars and light trucks equipped with a variety of PFI engine types

and sizes. These PFI vehicles produce much lower levels of PM emissions than the SIDI vehicles of the E-94-2 study, which is a key factor distinguishing EPAAct and E-94-2 studies.

The EPAAct fuels were blended to meet a design matrix of five variables as shown in Table 2-2. Aromatic content was considered at two levels: 15 vol% (a low aromatics fuel) and 35 vol% (a high aromatics fuel). Ethanol was considered at four levels: at the E0 and E10 levels, which are commonly found in the US market; and at the higher E15 and E20 levels. Two RVP levels were considered to include both summer and winter gasolines. Five and three levels were considered for T50 and T90, respectively. In total, 27 experimental fuels were created and tested for emissions in the fleet of 15 vehicles. However, not all combinations of the 240 possible design levels could be tested due to both practical and cost reasons.

Table 2-2
Design Levels for Fuels used in EPAAct

Factor	Number of Levels for Property	Design Values		
		Low	Middle	High
Aromatics (vol%)	2	15		35
Ethanol (vol%)	4	0	10, 15	20
RVP (psi)	2	7		10
T50 (°F)	5	150	165, 190, 220	240
T90 (°F)	3	300	325	340
Source: Table 2. EPAAct (2013a).				

The EPAAct study noted that “[a] critical point about the design of the program is that the properties of the test fuel are assigned so as to span the boundaries of in-use fuel properties. This approach is designed specifically to provide a basis for the development of statistical models capable of predicting emissions for the majority of in-use fuels....Test fuel parameter ranges were originally drafted to span roughly the 5th to 95th percentiles of survey results for US gasolines.”⁴

Given this approach, the EPAAct fuels are dissimilar by design to the experimental fuels in the CRC emission studies. They may also be less representative of *typical* commercial gasolines found in the market.

For EPAAct, the particulate and gaseous emissions of the vehicles were also measured at the SwRI laboratory in San Antonio, TX, using the LA92 test cycle and reported for the

⁴ EPAAct (2013a), pp. 14-15.

individual phases of the cycle and as LA92 weighted-averages. PM was measured along with gaseous emissions including THC, NMOG, NMHC, CO, NO_x, and CO₂.

2.2 Other SIDI Emissions Datasets

Two other PM emissions studies are used in this work to test how well the PME index for SIDI vehicles performed when applied to other datasets, which tested appreciably different experimental fuels. Both data sets are from small CRC test programs involving only four vehicles each. In both cases, the vehicles had been used in the E-94-2 study and so the datasets are not independent with respect to vehicles. Further information can be found in the CRC E-94-3 and CRC E-129 reports.

CRC E-94-3

Because the E-94-2 study had used experimental fuels that were blended to match design targets for ethanol (“match-blended”), a follow-on study was conducted to determine whether the method of ethanol blending had an effect on PM emissions. For E-94-3, four additional E10 fuels were created by splash-blending 10 vol% ethanol into retained samples of the four E0 fuels tested in E-94-2 (see Table 2-3). Thus, the gasoline hydrocarbons of the splash-blended E10 fuels were identical to the E0 base fuels except for dilution. No effort was made to control other properties of the resulting E10 fuels, which were generally more volatile and of higher octane than their E10 counterparts in E-94-2. Emissions testing was performed at SwRI using the LA92 cycle; both PM and PN emissions were measured along with a range of gaseous pollutants.

Table 2-3
Experimental Fuels used in CRC E-94-3

Fuel	Base Fuel	AKI	EtOH* (vol%)	PMI
C-E10	C	91.5	9.44	1.28
D-E10	D	91.1	9.71	2.45
G-E10	G	96.4	9.75	1.17
H-E10	H	96.0	9.88	2.32
* Based on ASTM D4815. Source: Table ES-1. CRC E-94-3 Report (2018).				

CRC E-129

Given the introduction of E15 in commercial gasolines, the E-129 study was conducted to determine the effect of higher ethanol blends and gasolines blended with two other oxygenates (i-Butanol and MTBE) on the exhaust emissions and fuel economy of SIDI vehicles. Four test vehicles were drawn from among those used in E-94-2 and tested on a group of seven fuels created by splash-blending three oxygenates into a low-PMI Fuel C

in sufficient volumetric quantities to achieve two different oxygen content levels for each oxygenate type (see Table 2-4). Emissions testing was performed at SGS Transportation (Aurora, CO) using the LA92 cycle; PM emissions were measured along with a range of gaseous pollutants.

Table 2-4
Experimental Fuels used in CRC E-129

	Oxygenate Type	Oxygen Content* (wt %)	PMI[†]
Fuel C	—	0.0%	1.30 [‡]
EtOH10	Ethanol	3.7%	1.16
EtOH15	Ethanol	5.5%	1.08
iBut16	i-Butanol	3.8%	1.07
iBut24	i-Butanol	5.6%	1.09
MTBE19	MTBE	3.5%	1.04
MTBE29	MTBE	5.3%	0.92
* Reported by Gage Products Company in Certificates of Analysis. [†] Determined by a CRC member company using the Honda PMI equation. [‡] Fuel was re-blended for this study to target the specifications of Fuel C in the CRC E-94-2 study. In E-94-2, the original Fuel C had a PMI of 1.40. Source: Table 8-1. CRC E-129 Report (2019).			

2.3 Yield Sooting Index (YSI) Data

One advance made in the PME formulation is the replacement of the $1 + \text{DBE}$ numerator in the Honda equation with an empirical formula called the *yTerm* that estimates each hydrocarbon compound's chemical propensity to form PM when combusted. The *yTerm* is derived from measurements of the Yield Sooting Index (YSI) developed by the Pfefferle Lab Group at Yale University.⁵ YSI is a standardized measure of soot formation that its authors developed from measurements of the soot formed when pure compounds are combusted in a methane diffusion flame. A focus of the YSI work has been characterizing the soot formation potential of bio-fuels, including many complex oxygenated compounds that these fuels may contain, which include ketones, aldehydes, and compounds with multiple oxygen groups.

The YSI Version 2 Database contains YSI values for some 441 compounds, including both low and high soot-forming compounds, when measured on a *weight* basis (a constant mass

⁵ Das 2017. The YSI Version 2 database can be found at <https://pfefferlehallerlabs.yale.edu/ysi-database>.

concentration in the methane flame). Of these, some 131 compounds are found in the gasolines tested in the several emission studies, while the remainder are not. Some 200 compounds are complex oxygenates that may be found in bio-fuels but are not found in commercial gasoline. This emphasis reflects an underlying motivation for the YSI work in support of research programs involving bio-fuels.

While the measured soot values pertain to combustion in a vaporized state, the YSI values should reflect the “stability” of the compounds’ bonds and give a *relative* measure of sooting potential when combusted in a motor vehicle. This is how it is used in the PME formulation.

2.4 Detailed Hydrocarbon Analysis of Fuels

2.4.1 ASTM and SSI DHA Methods

Both the Honda PMI and the PME index developed in this work require as inputs the detailed speciation of hydrocarbons present in the gasoline using one of two DHA methods. The result of a DHA analysis lists the hydrocarbons compounds detected in a fuel along with measures of its concentration (wt%, vol%, and mole%). Two different types of DHA are used here:

- ASTM DHAs defined by ASTM standards including ASTM D6729, ASTM D6730, and ASTM D6733. In addition to these, some laboratories have modified the gas chromatography libraries used for compound identification to increase the number and types of compounds that can be detected, thereby creating variants.
- SSI DHAs developed by Separation Systems Inc. (SSI, Gulf Breeze, FL) under CRC AVFL-29 that characterize high molecular weight compounds more completely than the ASTM procedures.

For purposes of this work, the main difference is in how completely the ASTM and SSI DHA methods characterize the high-molecular weight gasoline hydrocarbons present in a fuel. The SSI DHA is estimated to reduce the fraction of a gasoline sample that remains unidentified from approximately 5% with the ASTM DHA to 0.5% with the SSI DHA.

These methods differ in terms of the technical details associated with the analysis but not the fundamental analytical approach, which is based on gas chromatography (GC). The GC method uses a capillary column to separate the individual chemical compounds in a sample so that they can be identified and quantified by a flame ionization detector (FID) placed at the end of the column. The identification of a specific compound is made by comparing the amount of time required for each to elute from the column and reach the detector. The amount of the compound present in the sampler is determined by the output signal from the FID. The time required to pass through the column is referred to as the retention time.

As stated in the ASTM specifications that apply to DHA analysis:

Each eluting component is identified by comparing its retention time to that established by analyzing reference standards or samples under identical conditions. The concentration of each component in mass percent is determined by normalization of the peak areas after correction of selected components with detector response factors. The unknown components are reported individually and as a summary total. (ASTM D6729)

One concern is that the higher molecular-weight compounds that may be of particular relevance to PM formation tend to elute late in the GC process. Their elution may overlap with the elution of other compounds, making their identification and quantification impossible based solely on retention time. Such heavy hydrocarbon compounds not identified by the ASTM DHA method can make disproportionate contributions to PM emissions even if they make up only a small portion of a fuel.

In light of this, CRC conducted Project AVFL-29 with the goal of reducing the fraction of a gasoline sample that remains unidentified by individual compound. The AVFL-29 method was developed by using a mass spectrometer (MS) to improve the GC method's ability to identify specific higher molecular weight compounds from their retention time. MS identifies specific molecules from the fragments produced after their ionization when they pass through a magnetic field under specific conditions. The fragmentation patterns of specific compounds after ionization are generally known and can be used to identify specific chemical compounds. After the compounds and their retention times using MS were identified, that information was used to enhance the GC method's ability to identify higher molecular weight compounds.

It is important to recognize that the ASTM DHA method is currently performed in fuel laboratories under different ASTM standards and with varying local extensions that create more variants. In fact, the GC libraries at SwRI were modified at the end of the E-94-2 project to improve the characterization of some compounds in the experimental fuels, which then required re-processing of the FID output data for E-94-2.

For purposes of this work, the ASTM DHAs performed for the EPAAct study and for the later CRC PM emissions studies are taken as being equivalent in terms of hydrocarbon coverage. An effort was made to compare the coverage of the EPAAct DHAs done by SwRI a decade ago (c. 2010) to the coverage of the SwRI DHAs done in 2017-2018 for the later CRC studies. It is possible that the SwRI GC library was extended over time and it is known that modifications were made for the later CRC studies, but the changes cannot be tracked over time. Somewhat fewer hydrocarbon species are identified in the EPAAct DHAs, but this may simply reflect differences in the blend stocks used to create the fuels in comparison to those used in the fuels of E-94-2 and later studies. Thus, all ASTM DHAs were taken as equivalent for the purposes of this work.

With publication of the SSI method from the CRC AVFL-29 project, some research labs have modified their methods to incorporate improvements. This has led some

companies/organizations to use a “hybrid” method that lies between the latest ASTM standard and the complete SSI DHA method.

The PME formulation is defined here in two forms depending on DHA type. PME-A is the form to be used with ASTM-based DHAs. Here, “ASTM” is a generic label that covers different versions of the DHA method (including D6729, D6730, and D6733), but it is typified by ASTM D6730 as practiced in research laboratories during the period 2016-2018. Laboratories that use a method that is comparable in hydrocarbon coverage to that used by SwRI in the E-94-2 and E-94-3 projects should use PME-A; PME-B is the form to be used with SSI DHAs. Laboratories using this method, or ones that have incorporated most of the improvements made by SSI, should use PME-B.

Until an approach is found to assess and control for the comparability of DHA methods across laboratories, a laboratory that uses a “hybrid” method should adopt the PME-B formulation, but it must recognize that the values it computes will be understated to an unknown extent compared to the values that a true SSI DHA would give. Use of the PME-A formulation would lead to overstating the PME-A values.

2.4.2 CRC DHA Database

A significant effort in this project was the work needed to organize the published DHAs for all 66 of the experimental fuels into a consistent database. The DHAs were done over an extended period of time—from c. 2010 for the EPAAct DHAs to the 2017-2018 period for the DHAs of the CRC studies. While most were performed by SwRI, they are affected to some extent by differences over time in the master lists of compounds that could be recognized and for inputs on boiling points and vapor pressures. Further, various formats were used to report and/or publish the DHAs. The DHAs for some projects reported the inputs to the PMI calculation along with each compound’s contribution to PMI. Other studies reported only the content of individual hydrocarbons in the fuels (as wt% and other measures) and gave separate tabulations of the total PMI values for each fuel.

For the CRC AVFL-29 work, SSI created an expanded list of compounds that could be identified in gasoline along with updated values for boiling points and vapor pressures. Using this “master” list of compounds in gasoline⁶ as a starting point, the DHAs for each of the 66 experimental fuels were merged into the database. CAS numbers were used as unique identifiers when available and the compound name (text string) when not. Care was taken to add entries to the database for unique identifiers that were found in the DHAs but not in the master list. In some cases, this means a compound may appear more than once in the list if it was identified using a different name or with a different spelling in the DHAs. Finally, the YSI Version 2 database was merged with the DHA database by compound so that the Yield Sooting Index (YSI) could be used in this work as well.

The diversity of data sources and formats, along with the number (861) of hydrocarbons that are found in the experimental gasolines, made this a daunting task. A series of quality

⁶ See <http://crcsite.wpengine.com/wp-content/uploads/2019/05/HCE-Master-Database-for-CRC-Project-AVFL-29-2018MAY30-1.xlsx> for the AVFL-29 Master Database.

control steps were imposed to assure accuracy; the ability to replicate the Honda PMI values reported for the fuels in the original studies was the key test. The values for boiling point (BP) and vapor pressure (VP_{443K}) in the SSI master list of compounds were adopted as the standardized values when available except for the oxygenated compounds. For compounds that did not exist in the SSI master list, boiling points and vapor pressures were pulled from E-94-2/3, E-129, and EPAct, in that order.

Empirical (measured) vapor pressures must be used for oxygenated compounds found in gasoline because the correlation equation between VP_{443K} and BP given in Aikawa 2010 is valid only for non-oxygenated hydrocarbons. For oxygenates, VP_{443K} was standardized at the values reported by NIST as shown in Table 2-5 below. Note that i-Butanol and 2-methyl-1-propanol are equivalent compounds, but appear in the SSI Master List with separate vapor pressures. They were standardized to a single boiling point value in this study.

Table 2-5
Vapor Pressure for Oxygenates in Gasoline (kPa at 443K)

Adopted for RW-107-2		ASTM DHAs			SSI Master List and DHAs
Oxygenate	Standard Value NIST *	E-94-2/3	E-129	EPAct	
Ethanol	1,475	1,581	1,581	1,581	853
i-Butanol	403		442	481	352
2-methyl-1-propanol	403				403
MTBE	1,075		1,440		1,075
* Source: https://webbook.nist.gov/					

Appendix A contains a master list of hydrocarbon compounds to document the result of the effort to place the DHAs on a consistent basis and to standardize the inputs used to calculate the Honda PMI and PME. Potential users of PME should reference the master list as an aid to incorporating PME in their work.

Once all inputs were standardized, the Honda PMI was computed for each fuel and compared to the published values. The published values could be replicated to two decimal places in most cases and, where not, the differences observed were in almost all cases smaller than ± 0.02 . Where PMI values are cited here, they refer to the re-calculated values based on the standardized inputs. A supplementary PowerPoint presentation is available on the CRC website to document the DHA sources and standardized PMI values used in this work.

Section 3.2 describes the development of a reduced-form representation for YSI, the empirical measure of soot formation by individual hydrocarbons, developed by the Pfefferle Lab Group, based on counts for:

- The carbon and oxygen atoms in the molecule;
- The double bonds and equivalents found outside of any aromatic rings that may be present; and
- The number of Aromatic rings when present.

This information was added to the database to support the YSI analysis and can also be found in the Appendix A tabulation of the master list of hydrocarbons.

3. THE PME FORMULATION

The PME formulation was developed over the course of a year in a sequential process that started with the Honda PMI equation and moved in succession through a series of improvements. This section discusses the end-point of that process—the PME formulation—to explain its concepts and empirical underpinnings.

3.1 Overview

Equation 3-1 below gives the mathematical formulation of the PME index in comparison to the Honda PMI equation. In both cases, the summation is computed over the individual compounds i that are identified in the DHA for a fuel. As is customary, the wt% _{i} parameter is in percentage terms—1.0 wt% is written as 1.0 in calculations.

$$\text{PME} = \left(\frac{43.4}{\text{LHV}} \right) \cdot [N_{\text{TECH}} \cdot \sum_i \frac{\text{wt}\%_i \cdot y\text{Term}_i}{VP_i^{\alpha=f(\text{EtOH})}}]^\beta \quad (3-1)$$

$$\text{PMI} = \sum_i \frac{\text{wt}\%_i \cdot (1+DBE)_i}{VP_i} \quad (3-2)$$

The boxed portion of the PME formulation re-writes the summation of the Honda PMI to improve the characterization of each compound's propensity to form PM emission when combusted. Outside the summation term, a normalization factor N_{TECH} causes the PME and PMI values to coincide at an index value of 1.00⁷. This term varies between PFI and SIDI technology. The portion of PME in square brackets (“[...]”) can be viewed as an enhancement of the PMI equation and can be referred to as PMI_{YSI} to indicate it is based on YSI. Like the Honda PMI, it is defined to be proportional to a fuel composition's propensity to form PM on a weight basis—*per kg of fuel*.

Finally, PME adds a term in front that adjusts the propensity of the fuel *composition* to account for changes in the fuel's energy content and to reflect that more *kg*'s of a fuel must be burned to power a vehicle over a given test cycle or real-world trip if it has a lower energy content. In this case, a fuel's propensity to form PM emissions is more than just the propensity of its composition. Energy content is measured as Lower Heating Value (LHV) in units of MJ/kg of fuel. The reference value of 43.4 MJ/kg was chosen as representative of conventional or reformulated gasoline not containing ethanol or another oxygenate (GREET 2019).

⁷ That is, a fuel with a PME value of 1.00 can be expected to have Honda PMI of 1.00 as well.

Green font is used in Eq. 3-1 to show the terms of the PME formulation that are based on empirical evidence. Beyond N_{TECH} , which is a normalization factor, the empirical terms are the following:

- The $yTerm_i$ in the numerator estimates the propensity of an individual compound to form PM when combusted based on an analysis of the YSI Version 2 database. It is based on a statistical approximation to the measured YSI values that can be easily evaluated for any compound based on counts of double bonds and equivalents and of aromatic and other rings in its molecular structure. The $yTerm_i$ is proportional to the expected YSI value of each compound and, as it pertains to the hydrocarbon composition of the fuel, is the same in all versions of the PME index.
- The $1/VP^\alpha$ term is a generalization of the $1/VP$ term in the Honda PMI. It allows each compound's contribution to PM formation to vary from simple inverse-proportionality to vapor pressure. The α exponent depends upon a fuel's ethanol content. It is empirically estimated from analysis of PM emissions in the CRC E-92-2 study (for SIDI vehicles) and the EPAct study (for PFI vehicles) and differs substantially between SIDI and PFI technologies.
- The β exponent in the bracketed term controls the linearity of the PME formulation to PM emissions. PME was first developed for SIDI vehicles using the SSI DHAs to give the fullest characterization of hydrocarbon content. The α exponents in the denominator were empirically determined to yield a result of $\beta=1.00$ —that is, a linear relationship of PME with LA92 Phase I PM emissions.

When PME is evaluated using an ASTM DHA, the bracketed term is numerically smaller because ASTM DHAs have a reduced coverage of gasoline hydrocarbons. In this case, the α exponents from PME-B are retained and β was empirically determined to achieve linearity with LA92 Phase I PM emissions.

When evaluated with an ASTM DHA, the terminology PME-A is used here; when evaluated with an SSI DHA, PME-B is used. Potential users should note that this usage is in contrast to the preceding CRC RW-107 study, where PMI referred to the Honda PMI evaluated using an ASTM DHA and PMI-A referred to Honda PMI evaluated with an SSI DHA. The empirical underpinnings of the PME formulation are explained in the following sections.

3.2 The $yTerm$ Numerator based on YSI

3.2.1 Concepts Behind the $yTerm$

In the Honda equation, the $1 + DBE$ term represents, in a generalized sense, the difficulty of breaking a molecule's double and higher bonds, which can be thought of as its general "stability." The Double Bond Equivalent (DBE) simplifies multiple types of bonds—including double bonds, triple bonds (which are doubly weighted), and rings—into an

equivalent number of double bonds. Single bonds are not considered in this determination because of their ease of breaking. The leading term 1 represents a contribution from saturated compounds while DBE represents an additional contribution from non-saturated compounds. Compounds with a larger number of stable bonds (higher DBE) are more likely to form PM when combusted.

The Pfefferle Lab Group at Yale measured the soot formed by pure hydrocarbon compounds, including oxygenates, when combusted in a methane diffusion flame and used it to formulate the Yield Sooting Index (YSI) as a standardized measure of soot formation potential. The YSI Version 2 Database contains YSI values on a unified scale for both low and high soot-forming compounds on a *weight* basis (a constant mass concentration in the flame). While the measured soot values pertain to combustion in a vaporized state, they should reflect the “stability” of the compounds’ bonds and give a *relative* measure of sooting potential when combusted in the liquid state in a motor vehicle. This is how it is used in PME.

While hundreds of compounds have been measured, the YSI work was motivated in part by the need to characterize the sooting potential of bio-based and blended petroleum-biofuels. As a result, the YSI database contains many compounds that are not found in commercial gasolines today. In particular, the YSI database contains a large number of complex oxygenates such as ketones, aldehydes, and compounds with multiple oxygen groups. Figure 3-1 shows the limited overlap that the YSI database has with the hydrocarbon compounds identified in the DHAs for the experimental fuels in the emissions datasets. Only 131 of the 861 compounds in the experimental fuels are contained in the YSI database.

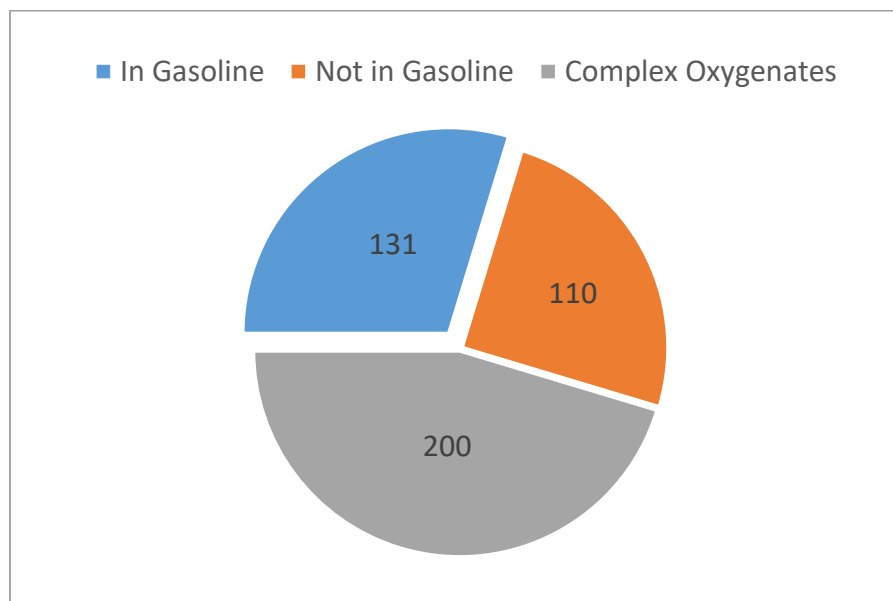
The YSI-based approach was adopted early in this work when it was not possible to gauge its ultimate success. While YSI can be estimated for compounds not in the database using an online calculator⁸, a statistical approximation was used to extrapolate the database to the full slate of hydrocarbons in the experimental fuels. The analysis was based on the 131 overlapping compounds in the YSI database that also are found in the experimental fuels.

3.2.2 Statistical Estimation of the *yTerm*

The Honda PMI builds certain assumptions into the $1 + \text{DBE}$ numerator about the relative contributions of saturated versus unsaturated compounds, specifically that all saturated compounds contribute in proportion to 1, while an unsaturated compound with 1 DBE contributes in proportion to 2 and a compound with 5 DBEs in proportion to 6. This assumption is replaced in PME with an empirical weighting of counts of single-bonds (SBs), of double bond equivalents (DBE), and of aromatic rings.

⁸ <https://ysi.ml.nrel.gov/>

Figure 3-1
Coverage of Gasoline Hydrocarbons in YSI Database



Outlined below are several points that became apparent during early phases of the statistical analysis.

- Saturated compounds with more carbon atoms have a higher YSI than saturated compounds with fewer carbons. The YSI values may be small in all cases, but saturated compounds are not all the same. The *size* of a molecule matters in the sense that more complex saturated compounds will have more single-bonds to break when combusted.
- In unsaturated compounds, the contribution of one DBE is the same whether it is found alone or in a *non-aromatic* ring. The convention is to count the double bonds present plus one additional DBE for each non-aromatic ring plus two additional DBE for each triple bond.
- In aromatic compounds, the first aromatic ring is responsible for a larger YSI contribution than a second or subsequent ring.

These findings led to the *yTerm* formulation shown below.

$$yTerm_i = (C+O-1) \cdot (A_0 + A_1 \cdot DBE_{NON} + A_2 \cdot ArRing_{FIRST} + A_3 \cdot ArRing_{ADD}) \quad (3-3)$$

The leading term C+O-1 is the measure of a molecule's "size" as it is the count of single bonds that would exist in a saturated molecule having the same Carbon+Oxygen Number (CON). Then, the coefficients A represent the YSI contributions:

- A_0 – per single-bond in the molecule.
- A_1 – an additional contribution per DBE not in aromatic rings (DBE_{NON}), meaning double bonds present (outside of *aromatic* rings) plus 1 for each *non-aromatic* ring present plus 2 for each triple bond present.
- A_2 – an additional contribution for the first aromatic ring ($ArRing_{FIRST}$)
- A_3 – an additional contribution for a second or subsequent aromatic ring ($ArRing_{ADD}$). These additional rings are counted the same regardless of whether the aromatic rings are fused together.

The rule for A_1 is followed even when aromatic rings are present in the molecule. For A_1 , the variable DBE_{NON} is the count of DBEs found outside of aromatic rings, while for A_2 and A_3 the variables $ArRing_{FIRST}$ and $ArRing_{ADD}$ are the counts of *rings*. DBEs within aromatic rings are not counted separately. Examples of these calculations are provided in Section 3.2.3.

The model of Eq. 3-3 was estimated using regression analysis for the dependent variable $YSI_{NORM} = YSI_i / (C+O-1)$ with independent variables of DBE_{NON} , $ArRing_{FIRST}$, and $ArRing_{ADD}$. Table 3-1 summarizes the statistical fit, which achieves an $R^2=0.90$ for the dependent variable. All of the A coefficients are highly significant statistically.

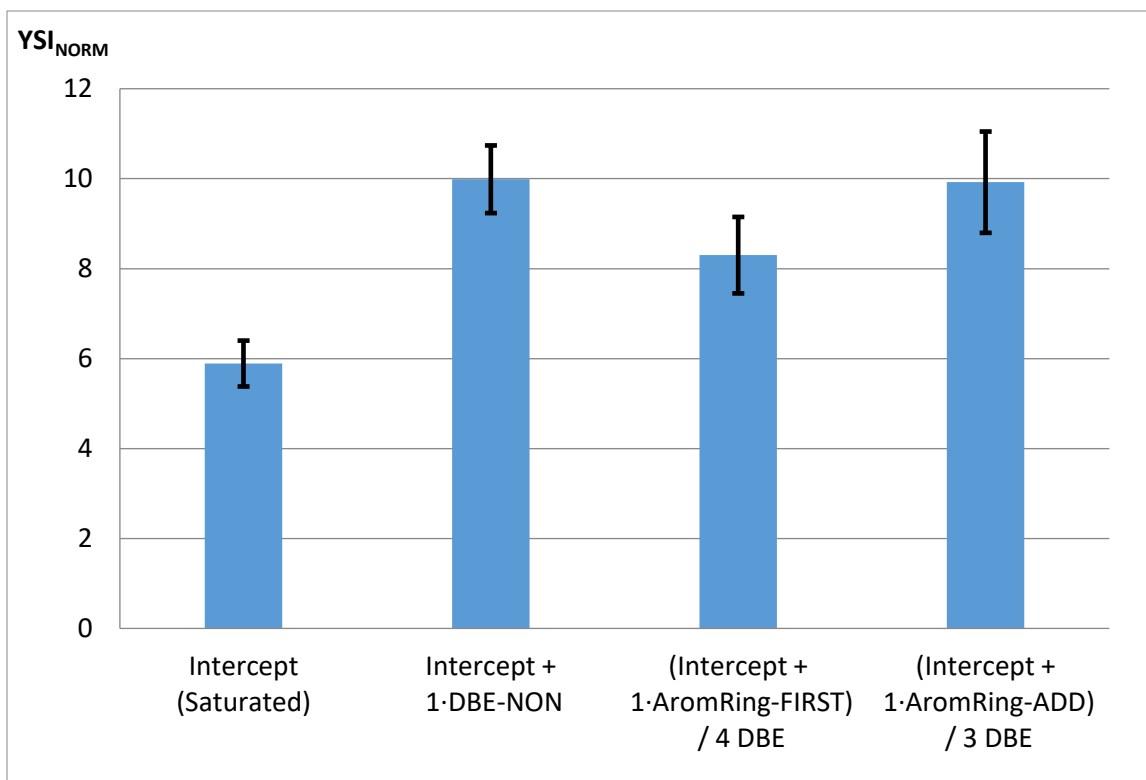
Table 3-1
Statistical Model of $YSI_{NORM} = YSI/(C+O-1)$

$YSI/(C+O-1) = A_0 + A_1 \cdot DBE_{NON} + A_2 \cdot ArRing_{FIRST} + A_3 \cdot ArRing_{ADD}$				
Term	Estimate	Std Err	Prob > t 	Normalized* Contribution to YSI_{NORM}
A_0 Intercept	5.89	0.51	<.0001	1.0
A_1 DBE_{NON}	4.04	0.68	<.0001	1.70 ± 0.23
A_2 $ArRing_{FIRST}$	27.3	1.0	<.0001	5.64 ± 0.53
A_3 $ArRing_{ADD}$	23.9	1.3	<.0001	5.05 ± 0.52
* The normalized contributions are defined as follows: $(A_0 + A_1)/A_0$ for DBE_{NON} ; $(A_0+A_2)/A_0$ for $ArRing_{FIRST}$; and $(A_0+A_3)/A_0$ for $ArRing_{ADD}$.				

The rightmost column gives the normalized contributions to YSI_{NORM} in a form that can be compared to the Honda PMI numerator $1 + DBE$. For saturated compounds, only the intercept pertains to the sooting potential. The intercept has a value of 1.0 when normalized as explained in the table, but it is now multiplied by the C+O-1 variable for “size” to give sooting potential. For unsaturated compounds, one DBE is now worth 1.7 times a single bond *before* its multiplication by C+O-1 for “size.” Aromatic rings are worth even more.

Figure 3-2 shows the empirical estimates for YSI_{NORM} on a per DBE basis. As expected from chemical principles, a DBE has more stability than a single bond (the intercept) and the same stability wherever found except in the first aromatic ring. A DBE alone, in a *non-aromatic* ring, or in a second or subsequent *aromatic* ring has the same YSI_{NORM} on a DBE basis. The first aromatic ring is the exception. It has greater stability in an absolute sense (see Table 3-1), but given its conventionally assigned 4 DBEs it has lesser stability per DBE than in subsequent aromatic rings (3 DBEs each). This result is also in agreement with expectations from chemical principles. Thus, the *yTerm* is structurally and directionally consistent with chemical principles and expectations, but with coefficients that are empirically derived.

Figure 3-2
Estimated Contributions to YSI_{NORM} on a DBE Basis

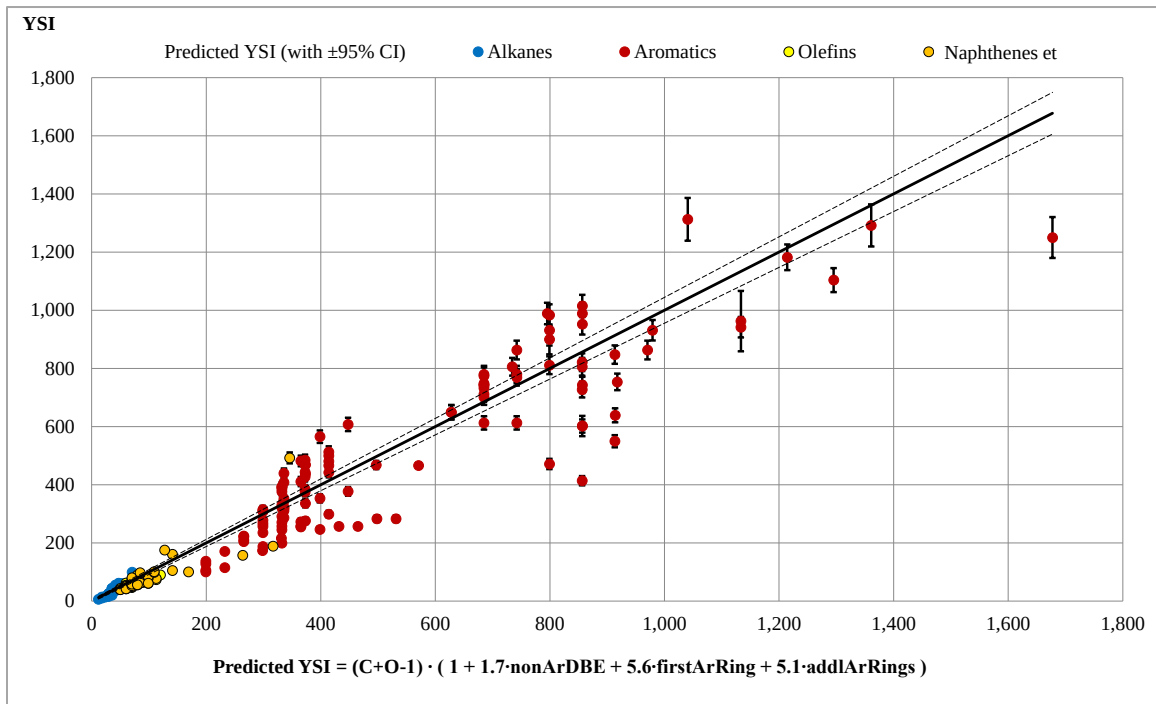


The *yTerm* in the numerator of PME is given in Eq. 3-4 where the A coefficients are rounded to one decimal in accord with the uncertainties cited in the previous table.

$$yTerm_i = (C+O-1) \cdot (1 + 1.7 \cdot DBE_{NON} + 5.6 \cdot ArRing_{FIRST} + 5.1 \cdot ArRing_{ADD}) \quad (3-4)$$

When scaled for size to the same basis as YSI, the *yTerm* proves to be a very good predictor of chemical sooting potential for the molecules (see Figure 3-3). The aromatic compounds have a pronounced scatter around the YSI model line, and one that is much greater than the uncertainty in the measured YSI values, while the scatter is much smaller for the other groups. Work by the YSI team indicates that this scatter is likely related to the internal structure and/or topology of the molecules that govern the order in which they break down into radicals during combustion (St. John 2017). This is a factor not accounted for in the PME formulation.

Figure 3-3
Comparison of YSI to Predictions based on the *yTerm*



The precision of PME could be improved if the *yTerm* were replaced by measured or estimated values for each compound, a task that was not undertaken in this project because the *yTerm* formulation was adopted at an early point in the work when the ultimate success of PME could not be known. Using measured/estimated values would reduce the scatter (hence, increase the precision), but it is not clear the extent to which it would improve the accuracy of PME for individual fuels because of the summation over many compounds. Doing so would also entail a cost and introduce the need for the maintenance, update, and distribution of a database to potential users. The current form of *yTerm* is one that can be documented in this report and applied by users on their own.

3.2.3 Sample Calculations and Data for the *yTerm*

This section presents three sample calculations for the *yTerm* so that its relationship to YSI and its calculation for use in the PME index are unambiguous. The examples range from the simple (ethanol, a C2 oxygenated molecule) to the complex (a C12 aromatic compound with two aromatic rings). For those wanting to implement similar calculations for their own fuels, Appendix A tabulates the counts of bonds and rings for the compounds found in the experimental fuels used here along with the calculated *yTerm* values and, where available, the measured YSI values.

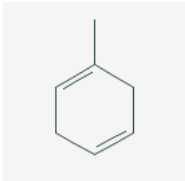
The first example, for ethanol, is given in Table 3-2. Ethanol is a saturated molecule with two carbons and one oxygen. Thus, its C+O-1 count is 2 and only the intercept term in the equation is used as it contains no rings. When computing a predicted YSI, one should use the estimated A coefficients found in the first column of Table 3-1; however, when computing *yTerm* for a PME calculation, one should use equation 3-4, which is based on the normalized coefficients from Table 3-1. For ethanol, the *yTerm* contribution of PME is 2, compared to 1 in the Honda Eq. The calculation predicts a YSI value of 12, which falls within the uncertainty in the measured YSI.

Table 3-2
Sample YSI and *yTerm* Calculation Number 1

Molecule: Ethanol (DBE=0) C2 Alkane, 1 oxygen. YSI = 10 ± 3
$ \begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{O}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array} $
Inputs: C+O-1=2. DBE _{NON} =0, ArRing _{FIRST} =0, ArRing _{ADD} =0.
Calculation:
$\text{YSI} = (\text{C}+\text{O}-1) \cdot (5.89 + 0.4.04 + 0.27.3 + 0.23.9) = 2 \cdot 5.9 = \mathbf{12}$
$y\text{-Term} = (\text{C}+\text{O}-1) \cdot (1 + 0.1.7 + 0.5.6 + 0.5.1) = 2 \cdot 1 = 2$

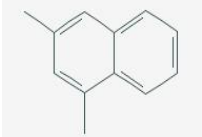
The second example is a C7 naphtho-olefin with double bonds and one non-aromatic ring (see Table 3-3). The determination of C+O-1 and relevant DBE and ring counts follows the same process used for ethanol. This molecule was chosen to illustrate that the non-aromatic ring is counted as a DBE on its own in addition to the two double bonds that it contains. The *yTerm* contribution to PME is 37. Here, the predicted YSI falls well below the measured value.

Table 3-3
Sample YSI and yTerm Calculation Number 2

Molecule: 1-methyl-1,4-cyclohexadiene C7 naphtho-olefin, no oxygen. YSI = 176 ± 8

Inputs: C+O-1=6. DBE _{NON} =2 + 1 non-aromatic Ring, ArRing _{FIRST} =0, ArRing _{ADD} =0.
Calculation:
$\text{YSI} = (\text{C}+\text{O}-1) \cdot (5.89 + 3 \cdot 4.04 + 0 \cdot 27.3 + 0 \cdot 23.9) = 6 \cdot 18.0 = \mathbf{108}$
$y\text{-Term} = (\text{C}+\text{O}-1) \cdot (1 + 3 \cdot 1.7 + 0 \cdot 5.6 + 0 \cdot 5.1) = 6 \cdot 6.1 = 37$

The final example is a C12 aromatic compound with two rings (Table 3-4). Here, the C+O-1 size is 11 with counts of ArRing_{FIRST}=1 and ArRing_{ADD}=1. The DBEs within the rings are not counted because the rings themselves have been counted. The *yTerm* contribution in PME is 129. The predicted YSI value of 628 falls below the measured value by about 15%.

Table 3-4
Sample YSI and yTerm Calculation Number 3

Molecule: 1,3-dimethylnaphthalene (DBE=7) C12 Aromatic, no oxygen. YSI = 743 ± 28

Inputs: C+O-1=11. DBE _{NON} =0, ArRing _{FIRST} =1, ArRing _{ADD} =1.
Calculation:
$\text{YSI} = (\text{C}+\text{O}-1) \cdot (5.89 + 0 \cdot 4.04 + 1 \cdot 27.3 + 1 \cdot 23.9) = 11 \cdot 57.1 = \mathbf{628}$
$y\text{-Term} = (\text{C}+\text{O}-1) \cdot (1 + 0 \cdot 1.7 + 1 \cdot 5.6 + 1 \cdot 5.1) = 11 \cdot 11.7 = 129$

3.3 The $1/VP^\alpha$ Denominator in PME

The authors of the Honda PMI noted that experimental evidence showed that the contribution of individual compounds was inversely proportional to their vapor pressure at 443K, but that the evidence did not give them a basis to select a specific functional form. The Honda Eq.'s denominator was made inversely proportional to VP_{443K} by assumption.

PME changes the denominator to allow an empirically determined exponent α to fine tune the role of vapor pressure. Vapor pressure spans more than three orders of magnitude across the compounds present in the experimental fuels—from a low of 3 kPa for some C12-14 hydrocarbons to a high of 16,957 kPa for propene. Given this wide range, a power-law relationship of the form $1/VP^\alpha$ was a logical and suitable choice.

The PME formulation is repeated in Eq. 3-4 below for reference in the following discussion. As one can see, the α coefficient is embedded in the denominator of each term in the summation. This means that it cannot be isolated by mathematical manipulation of the equation to permit estimation by the usual forms of regression analysis. Instead, an iterative method of estimation was used as described in Appendix B.

$$PME = \left(\frac{43.4}{LHV} \right) \cdot [N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}]^\beta \quad (3-4)$$

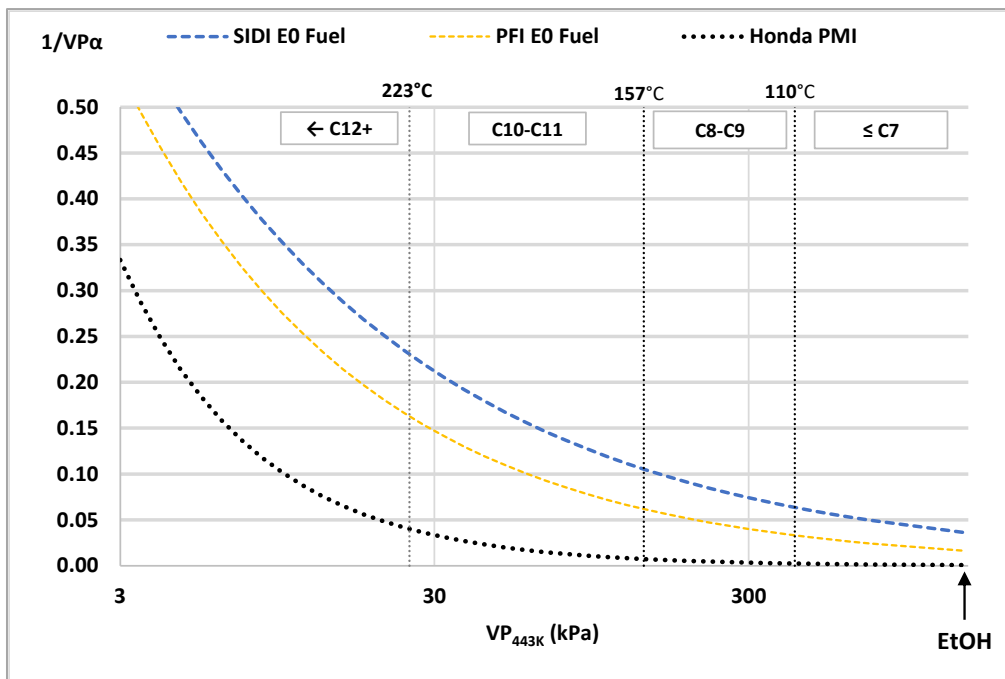
The objective in its determination is to find a value for α such that LA92 Phase I PM emissions of vehicles are linearly related to PME after accounting for the other effects present in Eq. 3-4, including the presence of ethanol. This means that the desired value of α should result in the coefficient β taking on the value 1.00 empirically. Once α has been determined, the constant N_{TECH} is determined so that PME coincides with the Honda PMI at a value of 1.00 to place both on a comparable scale.

At the outset, it was expected that α would depend on engine technology as PFI and SIDI vehicles differ greatly in the time allowed for injected fuel droplets to be heated and vaporized. PFI engines with fuel injection at the intake port during the intake stroke allow an extended time for droplets to vaporize and the fuel charge to mix before combustion begins. SIDI engines inject fuel directly into the cylinder during the combustion phase, giving much less time for vaporization and mixing. Thus, the α for PFI engines should be numerically larger and closer to the Honda Eq. $\alpha = 1$ than for SIDI engines.

As Figure 3-4 shows, these expectations are born out in the analysis. While the α value also depends on the ethanol content of the fuel, for simplicity only the values determined for the E0 fuels are shown here. The horizontal axis is VP_{443K} and extends on the right to the VP of ethanol itself. The vertical axis is the computed value of $1/VP^\alpha$, which can be thought of as indicating the enrichment of fuel droplets and localized rich areas in heavy hydrocarbons due to the early vaporization of the lighter compounds. The enrichment is relative to the overall hydrocarbon composition of the fuel. VP_{443K} is computed from the compounds' boiling points, except for the oxygenates which use empirical values. Vertical

lines are drawn to indicate the boiling point temperature ranges in which hydrocarbons of varying carbon number (CN) are typically found.

Figure 3-4
Relationship of $1/VP^\alpha$ to Engine Technology and the Honda PMI



The numerically smaller α found for SIDI engines indicates that a wide range of hydrocarbons contribute to PM formation although the heavy hydrocarbons with low vapor pressures make the largest contributions. Only small fractions of the lighter hydrocarbons remain in droplets and localized rich areas. The same is true in PFI engines, although the shift in contribution across the VP range makes the heavy hydrocarbons slightly less important in comparison to SIDI engines. Both empirical lines indicate greater contributions to PM formation by hydrocarbons across the range in VP, but they imply a larger relative contribution by the lighter compounds—even at boiling points of 100°C and below—compared to the Honda Equation.

The Honda Eq. shows no or very small contributions until the VP approaches 30 kPa. This is a fundamental difference in the attribution of responsibility for PM formation. The Honda Eq. attributes PM almost solely to heavy hydrocarbons. PME takes a more nuanced view in which the heavy hydrocarbons are most important, but some contributions are made along the full spectrum of VPs.

3.4 Energy Content Term

The leading term in PME represents the effect of varying energy content (due to fuel composition) on the PM emissions realized from a vehicle. Because the summation term

in PME gives a value stated on a weight basis—i.e., the fuel’s propensity to form soot per kg—the energy content term was introduced to account for the fact that more kilograms must be consumed if the energy content is lower. The numerator 43.4 MJ/kg is a reference value for energy content that is representative of conventional or reformulated gasoline without ethanol. In this study, with a few exceptions, only ethanol-containing fuels are appreciably lower than 43.4 MJ/kg.

The need for the term can be understood by a simple thought experiment. Assume for illustration that ethanol has no effect on PM emissions other than to dilute the gasoline hydrocarbons. If 10 wt% ethanol is added to an E0 gasoline, the PM formation potential is reduced by 10% per kg of fuel. However, the blended fuel will contain about 3.5% less energy than before so that $1/(1-0.035) = 1.036$ times as much blended fuel must be consumed to propel the vehicle over the drive cycle. Compared to PM emissions on the E0 fuel, the emissions from the blended fuel are reduced, not to 0.90 due to dilution, but to $(1-0.10) \cdot 1.036 = 0.93$ instead.

Individual vehicles may respond differently to fuels and may use some fuels more (or less) efficiently than others. In such case, the actual emissions change due to energy content will differ somewhat by vehicle. However, this is a *vehicle response* factor and not one that can be incorporated in an index describing *fuels*.

3.5 Summary

The PME formulation is intended for research use in understanding how fuel composition influences PM emissions from motor vehicles. Blenders will want a simplified form that does not require a DHA to guide fuel blending. In either case, one expects the relationship between PM emissions and PME for fuel *i* and vehicle *k* to be as follows:

$$PM_{i,k} = A_k \cdot PME_i = A_k \cdot \left(\frac{43.4}{LHV} \right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=\alpha_0 + \Delta\alpha \cdot EtOH_{vol\%}}} \right]^1 \quad (3-5)$$

where A_k is the PM emissions response coefficient of vehicle *k* to PME, or equivalently, the PM emissions of the vehicle for a fuel with PME = 1.00. The exponent to VP has been written out as $\alpha = \alpha_0 + \Delta\alpha \cdot EtOH_{vol\%}$ to allow for varying ethanol contents. The relationship between PM emissions and PME is one of direct proportionality (linearity). For fuels research, the emissions response factors A_k can be determined through emissions analysis, but for fuel blending they need not be known if the objective is to achieve percentage reductions in PME.

Table 3-5 lays out the elements of PM formation in vehicles to show where and how they are represented in Eq. 3-5. Two elements are vehicle factors that influence A_k (not PME) that must be accounted for in PM emissions analysis. Four are fuel factors that are accounted for in PME. The PME formulation accounts for the major elements of PM formation in vehicles as presently understood by the research community.

Table 3-5
PME and the Elements of PM Formation in Vehicles

Element	How Represented in PM Emissions Analysis and the PME Formulation	Discussion
Vehicle Factors (Accounted for in Emissions Analysis)		
Fraction of fuel in fuel droplets or localized rich air-fuel ratios during LA92 Phase I.	Intercept terms for the average emission levels of vehicles.	Differs between SIDI and PFI vehicles.
Vehicle efficiency varies per kg of fuel. Vehicle emissions response varies by fuel.	Intercept terms for the average emission levels of vehicles. Increased residual error in the emissions analysis.	Vehicle specific, if present.
Fuel Factors (Accounted for in PME Index)		
Chemical propensity of the fuel composition to produce soot.	YSI-based $yTerm$ in numerator.	Influenced by the mix of gasoline hydrocarbons and ethanol or other oxygenates.
Early vaporization of light compounds leaves fuel droplets and localized rich air-fuel ratios enriched in heavy compounds.	$1/VP^{\alpha}$ term through the α_0 coefficient for E0 fuels.	Differs between SIDI and PFI vehicles.
Cooling of the fuel charge resulting from ethanol's presence leads to further enrichment.	$1/VP^{\alpha}$ term through the $\Delta\alpha$ coefficient for E>0 fuels.	Differs between SIDI and PFI vehicles and as a function of ethanol content.
Reduced energy content per kg of fuel when ethanol or other oxygenates are present.	43.4/LHV term.	Permits PME to adapt to different oxygenates.

The $\Delta\alpha$ coefficient in $\alpha = \alpha_0 + \Delta\alpha \cdot EtOH_{vol\%}$ represents ethanol's cooling of the fuel charge that results from ethanol's own higher Heat of Vaporization compared to gasoline hydrocarbons and from its tendency to form near-azeotropes with gasoline hydrocarbons. The near-azeotrope formation accelerates the vaporization of fuel fractions and depresses front-end distillation temperatures in ethanol-containing fuels, which results in substantial cooling of the fuel charge. In turn, the cooling leaves the remaining fuel droplets and localized rich air fuel ratios enriched in heavy hydrocarbons.

At present, the $\Delta\alpha$ coefficient in $\alpha = \alpha_0 + \Delta\alpha \cdot EtOH_{vol\%}$ is used only for ethanol and not for other oxygenates. Oxygenates differ in their Heats of Vaporization and their ability to form

near-azeotropes and, thus, their tendency to influence fuel vaporization. The work reported in Fioroni 2019 illustrates these differences.

In the studies used here, only one (CRC E-129) examined other oxygenates (i-Butanol and MTBE). Its small test fleet and use of fuels with low PM formation potential does not permit a meaningful test of PME performance for the other oxygenates. When PME is applied to fuels blended from oxygenates other than ethanol, the $\Delta\alpha$ coefficient should be set to zero. If PM emissions data are available for the fuels, a test should be applied to determine whether the observed emissions level of such fuels are different from that indicated by PME.

4. PME-B INDEX FOR SIDI VEHICLES

4.1 Introduction

The mathematical formulation for PME was developed using the E-94-2 emissions dataset of SIDI vehicles and SSI DHAs. The resulting index is termed PME-B. This approach was taken because the SSI DHAs give the most complete characterization of hydrocarbon composition for the $yTerm$ in the numerator. Thus, estimation of the other empirical terms will be least affected by uncertainty in the knowledge of fuel composition.

Table 4-1 shows the PME-B formulation for SIDI vehicles with the empirical coefficients estimated highlighted in green font. Coefficient values are tabulated below. The $\alpha=f(EtOH)$ term in the denominator consists of the coefficients α_{E0} and α_{E10} pertaining to E0 and E10 fuel groups. As shown, it can also be written as a function of the ethanol content where $EtOH_{VOL\%}$ is the volume percent as a decimal fraction—i.e., 10 vol% ethanol is written as the decimal value 0.10.

Table 4-1
The PME-B Index for SIDI Vehicles

$PME-B = \left(\frac{43.4}{LHV} \right) \cdot [N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}]^\beta$ $\alpha = \{ \alpha_{E0}, \alpha_{E10} \}$ $f(EtOH) = \alpha_{E0} + (\alpha_{E10} - \alpha_{E0}) \cdot EtOH_{VOL\%}$ $LHV = \text{Lower Heating Value in MJ/kg}$							
$yTerm_i = (C+O-1) \cdot (1 + 1.7 \cdot DBE_{NON} + 5.6 \cdot ArRing_{FIRST} + 5.1 \cdot ArRings_{ADD})$							
Engine Technology	DHA Type	Designation	N_{TECH}	α_{E0}	α_{E10}	α_{E20}	β
SIDI	SSI	PME-B	0.00597	0.456	0.443	—	1.00
Note: Green font denotes empirically estimated parameters.							

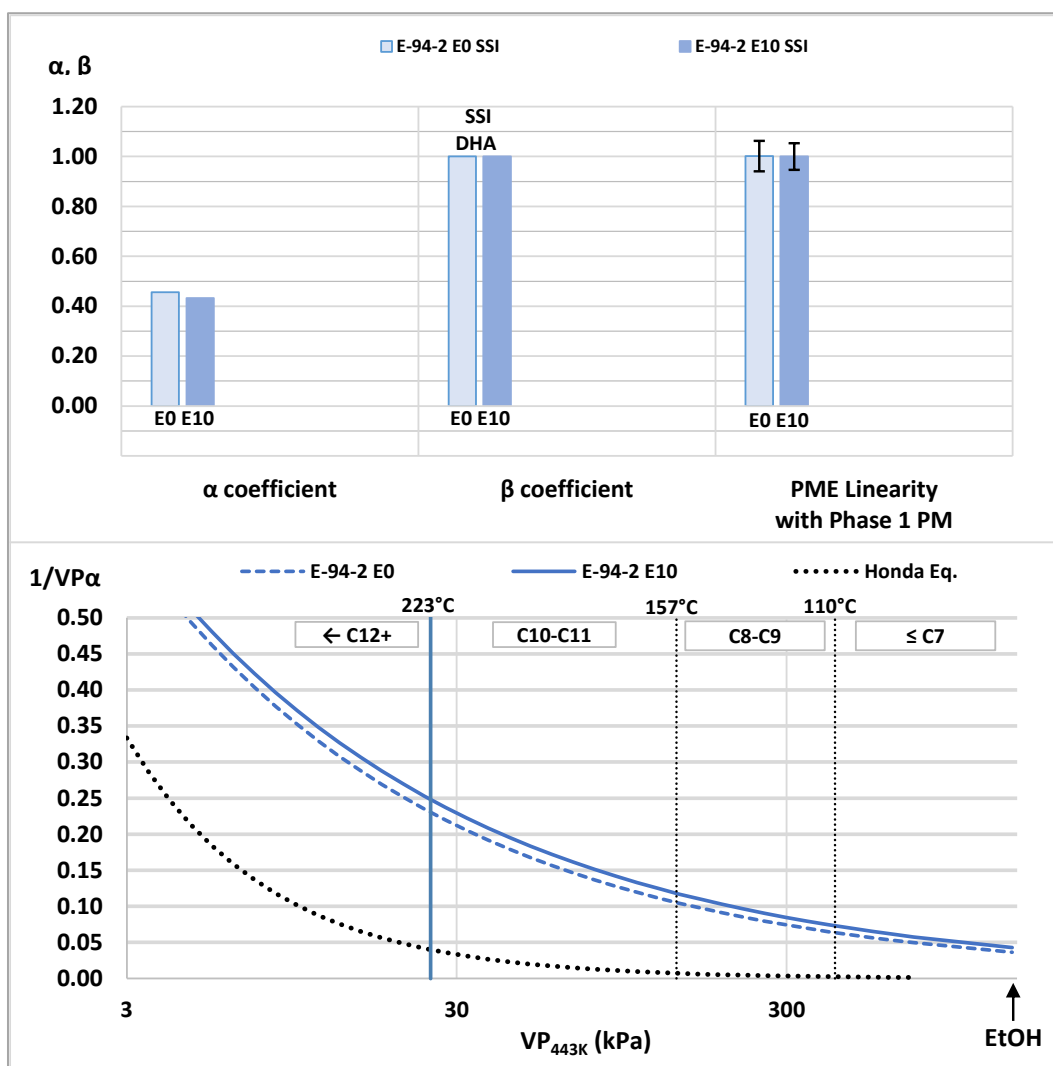
The α coefficients are determined in an iterative search to find values that cause PME-B to have a linear relationship with LA92 Phase I PM emissions in both the E0 and E10 fuel groups, meaning that $\beta=1.00$. The N_{TECH} coefficient is determined so that PME-B coincides with the Honda Eq. at the index value 1.00.

To calculate PME-B, one computes the term $\frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}$ for each compound in the SSI DHA and sums the values to a total for the fuel. The total is normalized by N_{TECH} and then taken as calculated because the coefficient β equals 1.00. Then, the value is multiplied by

the energy adjustment term $43.4/\text{LHV}$ to produce the fuel's PME-B index when used in SIDI vehicles.

Figure 4-1 graphs the coefficient values α and β and the implication of the α coefficients in the denominator. As shown at the right, the PME-B is linearly proportional to the LA92 Phase I PM emissions of the SIDI vehicles in the E-94-2 dataset for both E0 and E10 fuels to within uncertainties of $\pm 6\%$ and $\pm 5\%$, respectively.

Figure 4-1
PME-B Coefficients for SIDI Vehicles



The α_{E0} coefficient governs the vaporization line in the lower portion of the figure. The value $\alpha=0.456$ indicates that much larger portions of all hydrocarbons contribute to PM formation than the $\alpha=1.00$ value of the Honda Eq. Ethanol at the E10 level slightly reduces the α coefficient and shifts the $1/VP^\alpha$ term upward. This shift affects heavy hydrocarbons (with low VPs) by a larger amount than lighter compounds (with high VPs) and, thus,

increases the yield of PM from the heavier compounds. This is the first of ethanol's adverse impacts on PM emissions, with the second being a reduction in energy content.

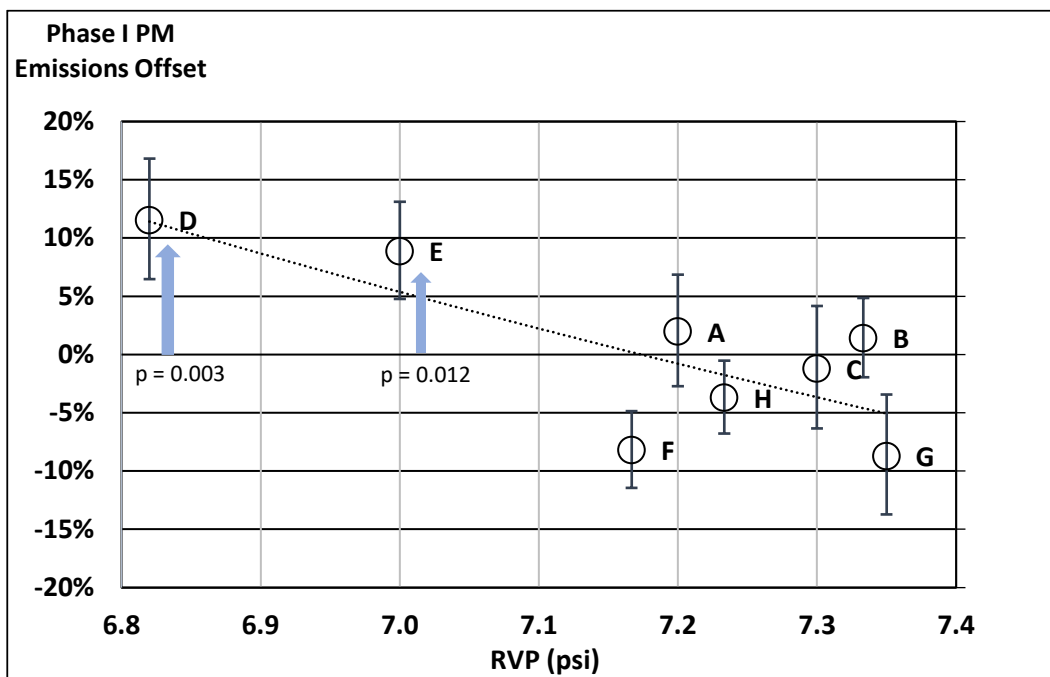
4.2 Performance of PME-B for SIDI Vehicles

4.2.1 Performance in the E-94-2 Dataset

Following estimation of the coefficient values, the PME-B index for SIDI vehicles was evaluated for completeness by examining the emissions residuals (observed minus predicted emissions) versus a series of fuel variables. The objective was to determine whether the index fit all fuels and whether other fuel properties would improve the index.

Figure 4-2 shows that the two fuels (D and E) in the E-94-2 dataset are offset from the PME-B index by statistically significant amounts. Fuel D is a High PMI regular-grade E0 while Fuel E is a Low PMI premium-grade E10. The two fuels stand apart from the others in having RVPs that are at or slightly below the RVP=7 psi target; all other fuels are clustered between 7.2-7.3 psi, slightly above the target.

Figure 4-2
LA92 Phase I PM Emission Residuals from PME-B for SIDI Vehicles by Fuel



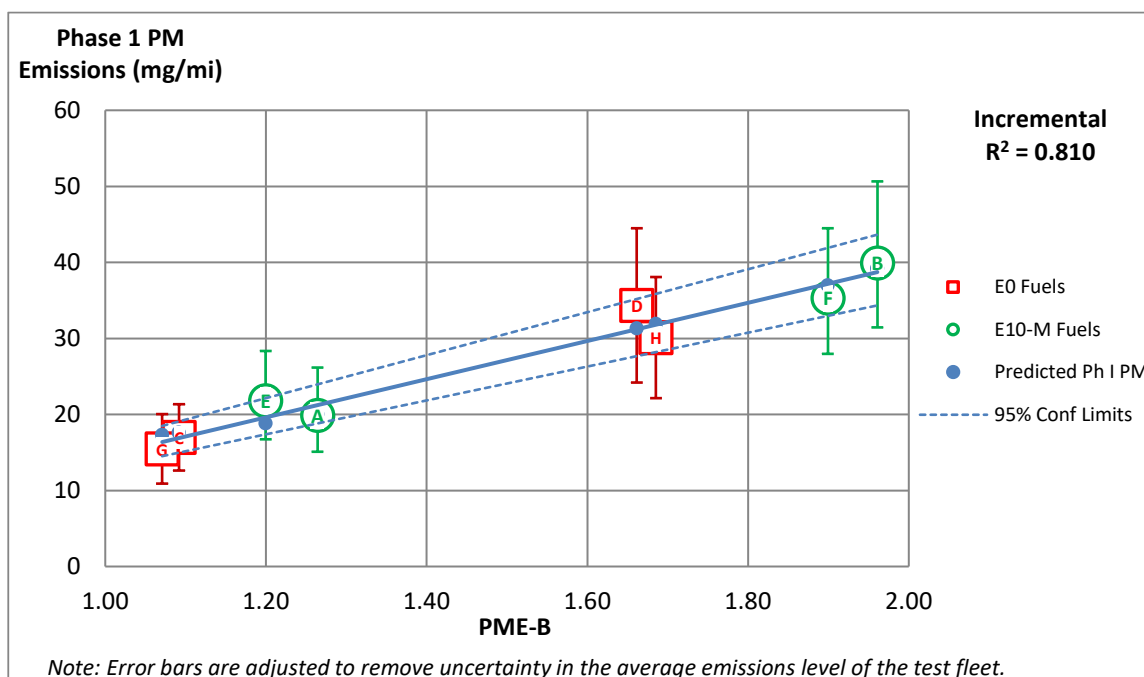
It is not known if the observed offsets are related to the RVP differences of the fuels. RVP proves to be a statistically significant predictor of the differences, but the fuels span a range of only ~0.5 psi and the possibility remains that the alignment is simply by chance. The bulk properties for fuels D and E were carefully examined to determine if any property would distinguish the two fuels from the others as a group. No candidates were found, and the cause of the observed offsets remains unexplained. This is the first time that a misfit

has been found for an individual fuel(s) in the PM emissions analysis of this and related datasets.

A parallel effort tested the PM emissions residuals against all available bulk fuel properties to see if the addition of another variable might improve PME-B. Both RVP and T05 at the front of the ASTM D86 distillation curve proved to be statistically significant. These are synonyms and also connected to the residual offsets observed for Fuels D and E. Neither were incorporated into the PME formulation because the available data are insufficient to give a definitive answer. No other variables from a list of some 20 bulk properties came close to statistical significance except for T60 and T70, which reached the $p=0.07$ level of significance. Such could be described as a “hint” of possible significance, but it falls far short of the $p=0.01$ level otherwise used throughout the work.

Figure 4-3 shows the performance of PME-B as a predictor of LA92 Phase I PM emissions in the E-94-2 dataset. In this, the overall trend of PM emissions with PME-B is plotted in blue and the average emission values by fuel are plotted in red and green. The error bars in the figure have been adjusted to remove the effect of uncertainty in the overall level of emissions (due to the finite number of measurements). This component of the uncertainty is shared by all values and simplify influences where the points and lines are plotted on the vertical axis. By removing this component, the adjusted error bars better indicate the uncertainty in the location of data points relative to the overall trend line with PME-B.

Figure 4-3
PME-B Performance in the E-94-2 Emissions Dataset



The linearity of LA92 Phase I emissions with PME-B is easily seen and the linearity holds for both E0 and E10 fuel groups. In contrast, the similar plot for PMI-A (see CRC RW-

107) shows an upward curving line with LA92 Phase I PM emissions from E10 fuels consistently above that from E0 fuels of comparable PMI. The observed ethanol bias in the Honda PMI is caused by the fact that it accounts for the dilution effect and low chemical sooting tendency (i.e., YSI) of ethanol, which are the benefits of ethanol blending, but not the two adverse effects—charge cooling and lower energy content—that PME accounts for as well.

Table 4-2 compares a series of performance measures for PME-B to measures for the Honda PMI-A⁹ from the RW-107 study. The PMI-A measures were calculated in RW-107 after it had been linearized by an empirically fit exponent. The performance differences would be much starker if PME-B were compared to PMI-A directly.

Table 4-2
PME-B Performance Measures for the E-94-2 Emissions Dataset

	PME-B This Study		Honda PMI-A* RW-107
Incremental R ²	0.810		0.777
r _{PEARSON}	0.98		n/a
ρ _{SPEARMAN}	0.95		n/a
Error Metric			
RMS Error	8%		11%
MAE	16%		22%
EtOH Bias	Percent	Prob> t	Percent
All Fuels	6%	0.09	18%
Low PMI	15%	0.006	22%
High PMI	-3%	0.42	11%
* After PMI was linearized by an empirically fit exponent in RW-107.			

The performance measures and error metrics are as follows:

- Incremental R² – the conventional R² value after removing the contribution to R² made by the different average emission levels of the vehicles has been removed. The Incremental R² measures the ability of the PM index (PME-B or PMI-A) to explain variation in LA92 Phase I PM emissions across fuels.
- r_{PEARSON} – the usual (Pearson) correlation coefficient *r* for the concordance of two variables in a dataset.

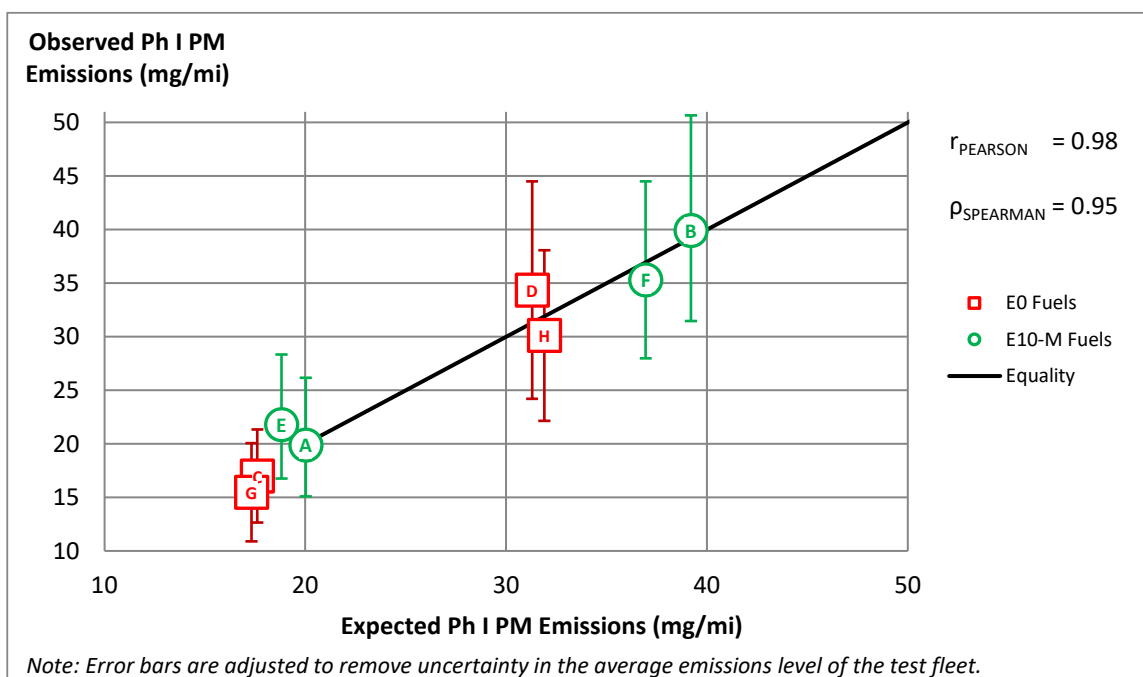
⁹ PMI-A refers to the Honda PMI evaluated using SSI DHAs.

- ρ_{SPEARMAN} – the Spearman correlation coefficient ρ for the ability of one variable to rank the values of another variable. This is the Pearson r applied to the ranks (1 to N) of each variable.
- RMS Error – the root-mean-square error measure for goodness of fit.
- MAE – the maximum absolute error observed.
- Ethanol bias – the percent difference on average between PM emissions for E10 and E0 fuels.

As can be seen, PME-B performs better than PMI-A in all respects. It explains a larger part of the emissions variation among fuels. Its RMS and MAE errors are reduced, and it is without an ethanol bias overall. The apparent significance of the ethanol bias in Low PMI fuels is directly related to Fuel E, which carries an unexplained fuel effect.

Further, PME-B does a good job of ranking fuels for emissions (see Figure 4-4). Its high r_{PEARSON} and ρ_{SPEARMAN} values indicate its predictive power. For ranking, some errors will be made—such as placing Fuel E at higher emissions than Fuel A, and Fuel D at higher emissions than Fuel H. But it should be noted that there is inherent uncertainty in the ranking of fuels close in measured PM emissions, as indicated by the error bars, and that the ranking errors involve the two fuels (D and E) for which unexplained offsets were observed.

Figure 4-4
Ranking of Fuels for Emissions using PME-B for SIDI Vehicles



All of the performance measures would be improved if the cause for offsets in Fuels D and E could be identified and incorporated in the PME formulation. The fuel data points in

Figure 4-3 would cluster closer to the line, the ethanol bias would vanish in both Low and High PMI groups, and the ranking errors would be reduced as well.

4.2.2 Performance in Other Datasets

The performance of PME-B was examined in two other datasets from recent CRC projects on PM emissions. The datasets are small, involving only four vehicles each, and are not fully independent because the vehicles were drawn from the test fleet used in E-94-2. Further validation of the PME-B index is needed in future work.

E-94-3 Emissions Dataset

The E-94-3 study examined whether the method of blending E10 fuels influenced PM emissions. Four E10 fuels were created by splash-blending ethanol into the four E0 fuels of the E-94-2 study. Other properties of the splash-blended E10 fuels—specifically AKI and RVP—were allowed to vary freely and differ from the values of the match-blended E10 fuels in E-94-2.

Figure 4-5 and Table 4-3 illustrate that the PME-B index does not improve on the performance of the PMI-A index seen in RW-107. In the figure, the splash-blended E10 fuels are labeled as E10-S. LA92 Phase I PM emissions are linearly related to PME-B overall, but the ethanol bias between E10-S and E0 fuels remains despite the improvements made in PME-B. The chief conclusion drawn in E-94-3 (see Table 4-4) was that splash blending increased LA92 Phase I PM emissions overall and by a statistically significant amount in the Low PMI fuels, a conclusion not dependent on a PM index in any way.

Figure 4-5
PME Performance in the E-94-3 Emissions Dataset

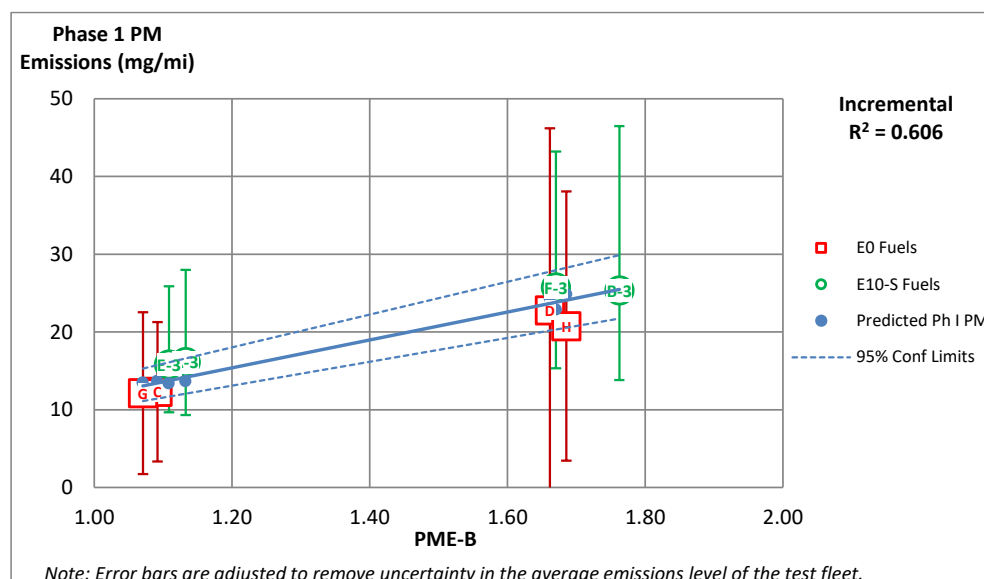


Table 4-3
PME-B Performance Measures for the E-94-3 Emissions Dataset

	PME-B This Study		Honda PMI-B* RW-107
Incremental R ²	0.606		0.618
r _{PEARSON}	0.98		n/a
ρ _{SPEARMAN}	0.71		n/a
Error Metric			
RMS Error	14%		14%
MAE	20%		23%
EtOH Bias	Percent	Prob> t	Percent
All Fuels	26%	0.0009	24%
Low PMI	31%	0.009	27%
High PMI	20%	0.05	22%
* After PMI is linearized by an empirically fit exponent.			

Table 4-4
Model-Estimated LA92 Phase 1 PM Emissions Change for E0→E10-S.
Honda PMI with SSI DHAs

	Four-Vehicle Group	
	Emissions Change	Statistical Significance
Average of All Fuels	<u>+24%</u>	p = 0.002
Avg Low PMI	<u>+31%</u>	p = 0.006
Low AKI / Low PMI	<u>+31%</u>	p = 0.043
High AKI / Low PMI	<u>+31%</u>	p = 0.046
Avg High PMI	+17%	p = 0.086
Low AKI / High PMI	+11%	p = 0.41
High AKI / High PMI	+24%	p = 0.10
Note: Underlining indicates that the estimated change is statistically significant at the p ≤ 0.05 level. Underlining with bold italicized text indicates the change is statistically significant at the p ≤ 0.01 level. Source: Table 24 of CRC RW-107.		

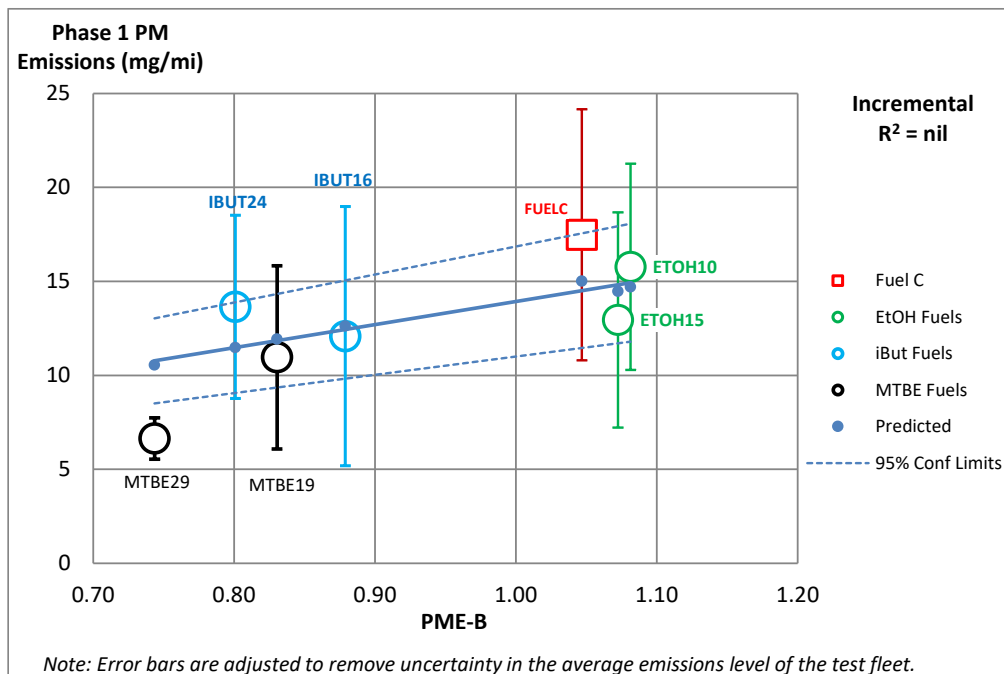
The same result is seen here. Splash-blending of ethanol increases the quantity of fuel that vaporizes at low boiling points compared to the base fuels. This appears to lead to a greater cooling effect compared to the match-blended base fuel, which holds the fuel fraction at low boiling points to only that needed for the targeted RVP level.

E-129 Emissions Dataset

The E-129 study examined PM and gaseous emissions from fuels splash-blended with ethanol, i-Butanol, and MTBE at two levels of oxygen content equivalent to that reached in E10 and E15 gasoline. The base fuel was a low PMI Fuel C similar to that used in E-94-2. The PME-B index was computed with the $\Delta\alpha$ cooling effect considered only for the ethanol fuels.

As Figure 4-6 shows, there is little to be learned from this dataset about performance of PME-B. The Honda PMI and the PME-B levels of the oxygenated fuels are very low compared to the other datasets because of the greater dilution of the low PMI base fuel with oxygenates that themselves have very low propensity to form soot. Oxygenates formed up to 15% of the ethanol fuels, up to 24% of the i-Butanol fuels, and up to 29% of the MTBE fuels.

Figure 4-6
PME Performance in the E-129 Emissions Dataset



Recent work (Fioroni 2019) demonstrates empirically that the cooling effect of common alcohols differs greatly by alcohol in terms of both magnitude and the rate at which it is realized during fuel vaporization. Ethanol and methanol had large and early cooling

effects, while other alcohols (including i-Butanol) had smaller and delayed cooling effects; MTBE was not tested. To use PME-B with other alcohols it is best, at present, to account for the difference in energy content and to assume that no cooling effect is present. A larger dataset on other oxygenates, in fuels with high PM formation potential, will be needed to understand how to account for other oxygenates in the PME-B formulation.

4.3 Discussion

The performance analysis demonstrates that PME-B is an effective indicator of LA92 Phase I PM emissions and is without bias when used to compare finished gasolines of RVP~7 psi for use in SIDI vehicles. It is also complete in the sense that no other fuel property can be shown to add explanatory power for PM emissions with the currently available data. However, its performance is subject to two important caveats:

- The significance of PM emission residuals for Fuels D and E suggests that more might be learned about the fuel characteristics that influence PM emissions. The unexplained cause leading to PM emissions from these fuels being higher than indicated by PME-B could result from a number of possibilities. It could be an effect related to RVP within the narrow range of ~0.5 psi; differences in the total Heat of Vaporization of compounds at the front of the distillation curve and, thus, charge cooling; mid-range volatility (T60-T70); or even a distinctive response by some of the test fleet to unidentified characteristics of the two fuels.
- The performance on fuels from the E-94-3 study says that use of PME-B must be restricted to fuels blended to the same RVP level—specifically, RVP~7 psi based on the data available from E-94-2. It cannot be used in its current form to guide blending of ethanol into BOBs in a manner sensitive to achieving PM emission reductions.

CRC plans further work to examine PME-B using SIDI vehicles tested with new fuels to provide a stronger validation of PME-B. Among other things, it should be possible to determine its applicability to winter-grade gasolines. Further work is also needed to understand why splash-blending of ethanol leads to increased PM emissions. One likely hypothesis is that such fuels have a larger fuel fraction that evaporates early, leading to a larger cooling effect. If so, such an effect might be incorporated through a revised and more general $\Delta\alpha$ term in the exponent of VP in the denominator. At present $\Delta\alpha$ is restricted to ethanol content.

5. THE PME-A INDEX FOR SIDI VEHICLES

5.1 Development of the PME-A Formulation for SIDI Vehicles

The ASTM DHA procedure yields a subset of the information on a fuel’s hydrocarbon composition that is more completely determined in the SSI DHA. Use of the ASTM DHA to evaluate the summation term in PME yields a smaller numerical result because fewer hydrocarbon terms are included with, on average, lower propensities to soot ($yTerm_i$). Thus, the PME formulation evaluated with ASTM DHAs will give lower PME-A values and cannot be a linear indicator of LA92 Phase I PM emissions. Further, a PM emissions analysis based on ASTM DHAs cannot add anything new to the understanding of how the PME formulation accounts for PM emission.

Because of these limitations, a decision was made to “map” the PME-A formulation into the PME-B model to avoid creating a second set of α coefficients, when only a single set should exist for an engine type, whether SIDI or PFI. The approach taken was to retain the empirical coefficients in PME-B for SIDI vehicles—specifically, N_{TECH} and $\alpha = f(EtOH)$ —while estimating an exponent $\beta > 1.00$ to account for the lesser coverage of hydrocarbons in ASTM DHAs. Table 5-1 illustrates this.

Table 5-1
Applying the PME-B Formulation to ASTM DHAs for SIDI and PFI Vehicles

PME-B for SIDI Vehicles (SSI DHA)	$PM_{PhI} = A_{VEH} \cdot \left(\frac{43.4}{LHV} \right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}} \right]^{\beta=1}$
PME-A for SIDI Vehicles (ASTM DHA)	$PM_{PhI} = A_{VEH} \cdot \left(\frac{43.4}{LHV} \right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}} \right]^{\beta=1.17}$
Note: Green font denotes empirically estimated parameters.	

When estimated in this manner, PME-A for SIDI vehicles achieves (by design) nearly the same level of performance as PME-B. For this reason, the section does not show or discuss the performance measures for PME-A.

Table 5-2 compares the coefficients for PME-A for SIDI vehicles with those for PME-B. As shown, all empirical coefficients are carried forward from PME-B, except that β has been estimated to have a value of 1.17 to map the summation term calculated from ASTM

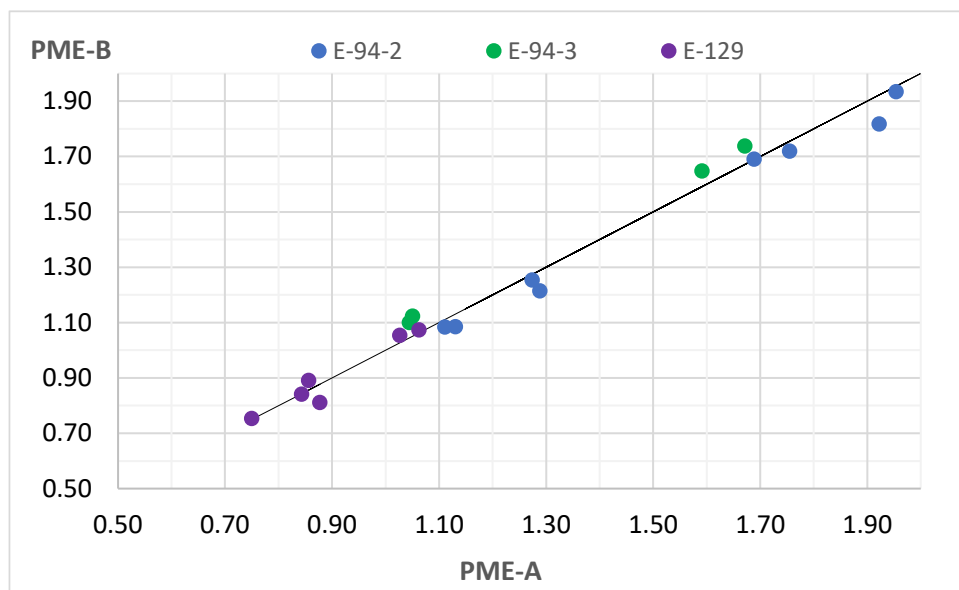
DHAs into its equivalent as calculated from SSI DHAs. Note that β applies to the entire term in square brackets. Once the bracketed term is exponentiated, it is then multiplied by the energy content term.

Table 5-2
The PME-A Formulation for SIDI Vehicles

$\text{PME} = \left(\frac{43.4}{\text{LHV}} \right) \cdot \left[N_{\text{TECH}} \cdot \sum_i \frac{\text{wt}\%_i \cdot y_{\text{Term}_i}}{v_{P_i}^{\alpha=f(\text{EtOH})}} \right]^\beta$ $\alpha = \{ \alpha_{\text{E0}}, \alpha_{\text{E10}} \}$ $f(\text{EtOH}) = \alpha_{\text{E0}} + (\alpha_{\text{E10}} - \alpha_{\text{E0}}) \cdot \text{EtOH}_{\text{VOL}\%}$ LHV = Lower Heating Value in MJ/kg							
$y_{\text{Term}_i} = (\text{C} + \text{O} - 1) \cdot (1 + 1.7 \cdot \text{DBE}_{\text{NON}} + 5.6 \cdot \text{ArRing}_{\text{FIRST}} + 5.1 \cdot \text{ArRings}_{\text{SADD}})$							
Engine Technology	DHA Type	Designation	N_{TECH}	α_{E0}	α_{E10}	α_{E20}	β
SIDI	ASTM	PME-A	0.00597	0.456	0.443	—	1.17
	SSI	PME-B	0.00597	0.456	0.443	—	1.00
Note: Green font denotes empirically estimated parameters.							

When estimated as described, the PME-A index for SIDI vehicles achieves, by design, essentially the same level of performance as PME-B. The close concordance between PME-A and PME-B values can be seen in Figure 5-1 and this must lead to closely comparable performance.

Figure 5-1
Concordance of PME-A and PME-B Values



5.2 Discussion

PME-A index with data for SIDI vehicles is subject to the same caveats as for PME-B:

- Its use must be restricted to fuels blended to the same RVP level—specifically, RVP~7 psi based on the data available from E-94-2.
- It cannot be used in its current form to guide blending of ethanol into BOBs in a manner sensitive to achieving PM emission reductions.

It is subject to one additional caveat—related to the design of the E-94-2 fuels for high versus low PM emissions potential—that can be tested when data on new fuels become available.

In the preceding RW-107 study, it was demonstrated that the Honda PMI gave essentially the same performance as a predictor for PM emissions regardless of the DHA type used.¹⁰ This outcome was initially puzzling as the SSI DHA had been developed specifically to improve the characterization of the heavy hydrocarbons that might make disproportionate contributions to PM formation. The comparable performance should be understood as a consequence of how the E-94-2 fuels were blended.

The Honda PMI was controlled to two different levels by adjusting the fuel fractions at the end of the distillation curve, while holding the aromatics content of the fuel nearly constant at ~25 vol%. Thus, the E-94-2 fuels have only one degree of freedom in how PMI was varied. If only one heavy blend stock was used to achieve this, as seems likely, then the PMI values of the fuels will be highly correlated with the PMI-A values based on the SSI DHAs. In this case, the SSI DHAs add additional information on fuel composition beyond that contained in the ASTM DHAs, but the information does not lead to improved predictive power for PM emissions because of the correlation.

The same will not necessarily be true when the PME formulation is applied to other fuels. The EPAct study, for example, changed both aromatics content and T90 as design variables. Thus, it has two degrees of freedom in how the PM propensity of fuels was varied. One *might* find clear evidence of a benefit from the enhanced CRC AVFL-29 procedure if SSI DHAs were available for the EPAct fuels.

¹⁰ See Section 5.3 of CRC RW-107 (2019) for a discussion of the PMI versus PMI-A comparison (ASTM versus SSI DHAs).

6. THE PME-A INDEX FOR PFI VEHICLES

6.1 Development of PME-A for PFI Vehicles

Development of PME-A for PFI vehicles takes the final step in the process illustrated in Table 6-1. The PME-A analysis for SIDI vehicles determined that the summation term in PME based on ASTM DHAs should be increased by 17% ($\beta=1.17$) in order to map into the PME-B values based on SSI DHAs. As this is a correction for the enhanced hydrocarbon coverage of SSI DHAs, the same was applied to the ASTM DHAs for the EPA experimental fuels. Thus, the $\beta=1.17$ coefficient is adopted and the other empirical terms are re-estimated to account for the large differences in fuel intake, vaporization and combustion compared to SIDI vehicles.

Table 6-1
Adapting the PME Formulation to PFI Vehicles with ASTM DHAs

PME-B for SIDI Vehicles (SSI DHA)	$PM_{PhI} = A_{VEH} \cdot \left(\frac{43.4}{LHV} \right) \cdot \left[\underbrace{N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}}_{\text{green font}} \right]^{\beta=1}$
PME-A for SIDI Vehicles (ASTM DHA)	$PM_{PhI} = A_{VEH} \cdot \left(\frac{43.4}{LHV} \right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}} \right]^{\beta=1.17}$
PME-A for PFI Vehicles (ASTM DHA)	$PM_{PhI} = A_{VEH} \cdot \left(\frac{43.4}{LHV} \right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}} \right]^{\beta=1.17}$
Note: Green font denotes empirically estimated parameters; red font denotes parameters adopted from prior formulations.	

Table 6-2 gives the PME-A index for PFI vehicles with the empirical coefficients highlighted in green and tabulated in comparison to the coefficients for SIDI vehicles. The $\alpha=f(EtOH)$ term in the denominator now consists of three coefficients: α_{E0} , α_{E10} , and α_{E20} pertaining to the EPA E0 through E20 fuel groups. The α_{E15} coefficient is treated as lying half-way between α_{E10} and α_{E20} . The function $f(EtOH)$ is now written in a more generalized form $\alpha_{E0} + \Delta\alpha \cdot EtOH_{VOL\%}$. As will be shown below, the $\Delta\alpha$ coefficient must be calculated in piecewise linear form with different slopes between E0→E10 and E10→E20. As before, $EtOH_{VOL\%}$ is the volume percent as a decimal fraction—i.e., 10 vol% ethanol is written as the decimal value 0.10.

Table 6-2
The PME-A Index for PFI Vehicles

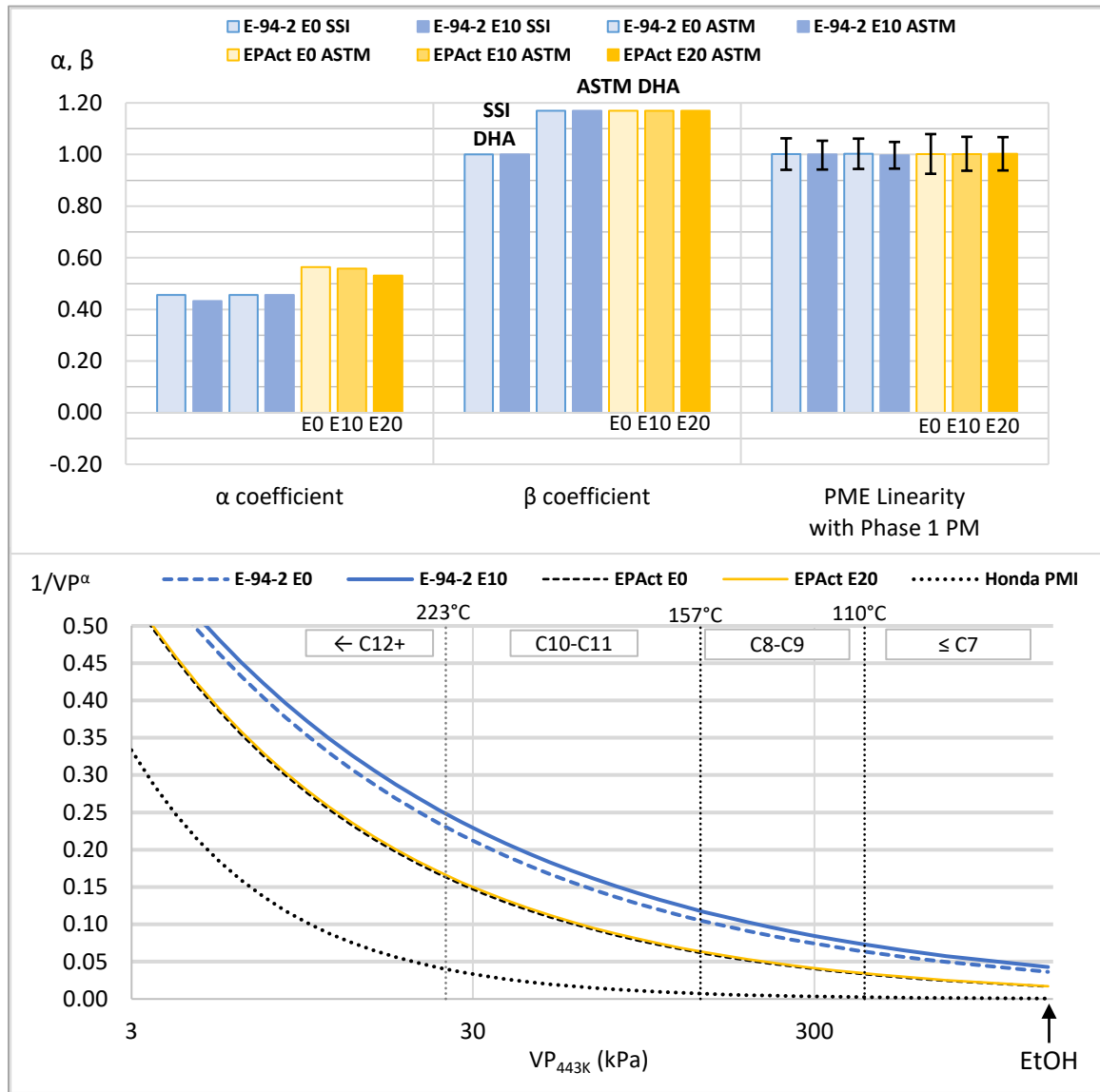
$\text{PME-A} = \left(\frac{43.4}{\text{LHV}} \right) \cdot [\textcolor{green}{N}_{TECH} \cdot \sum_i \frac{\text{wt}\%_i \cdot \textcolor{green}{yTerm}_i}{VP_i^{\alpha=f(\text{EtOH})}}]^{\beta=1.17}$ $\alpha = \{ \alpha_{E0}, \alpha_{E10}, \alpha_{E20} \}$ $f(\text{EtOH}) = \alpha_{E0} + \Delta\alpha \cdot \text{EtOH}_{\text{VOL}\%}$ LHV = Lower Heating Value in MJ/kg							
$yTerm_i = (C+O-1) \cdot (1 + 1.7 \cdot \text{DBE}_{\text{NON}} + 5.6 \cdot \text{ArRing}_{\text{FIRST}} + 5.1 \cdot \text{ArRings}_{\text{ADD}})$							
Engine Technology	DHA Type	Designation	N _{TECH}	α _{E0}	α _{E10}	α _{E20}	β
SIDI	ASTM	PME-A	0.00597	0.456	0.443	—	1.17
	SSI	PME-B	0.00597	0.456	0.443	—	1.00
PFI	ASTM	PME-A	0.0109	0.564	0.558	0.531	1.17
	SSI	PME-B	no data are presently available				
Note: Green font denotes empirically estimated parameters.							

The table notes that no data are presently available to develop a PME-B index for PFI vehicles. If and when such data become available, the starting point for further development work will be a PME-B index that adopts the N_{TECH}, α_{E0}, α_{E10}, and α_{E20} coefficients from PMI-A but sets the β coefficient to 1.00. Future analysis based on a suitable dataset containing SSI DHAs for the fuels could result in a new set of the coefficients for both PME-A and PME-B.

To calculate PME-A for PFI vehicles, one computes the term $\frac{\text{wt}\%_i \cdot yTerm_i}{VP_i^{\alpha=f(\text{EtOH})}}$ for each compound in the ASTM DHA and sums the values to a total for the fuel. Once multiplied by N_{TECH}, the value is exponentiated by β=1.17 which increases the total by 17%. Then, the value is multiplied by the energy adjustment term 43.4/LHV to produce the fuel's PME-A index when used in PFI vehicles.

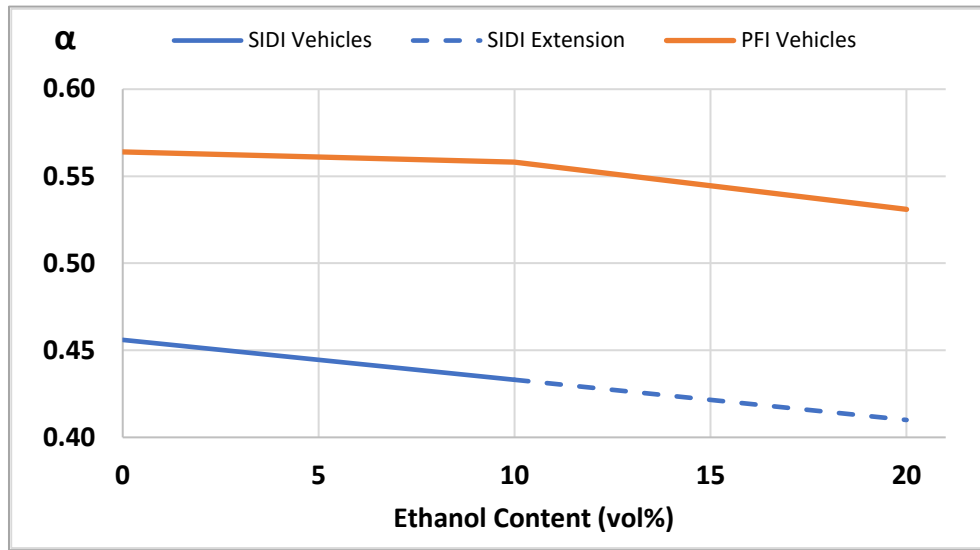
Figure 6-1 graphs the coefficient values α and β and the implication of the α coefficients in the denominator. As shown at the right, the PME-B is linearly proportional to the LA92 Phase I PM emissions of the PFI vehicles for each subgroup of fuels in the EPAAct dataset. The uncertainties in the linearity of PME-A with emissions range from ±6% to ±8%%. The α_{E0}=0.564 coefficient places the PFI vaporization line in the lower portion of the figure (dashed black line) at an intermediate location between the Honda Eq. at α_{E0}=1 (black dotted) and the PME-B index for SIDI vehicles at α_{E0}=0.456 (blue dashed). Remarkably, the influence of ethanol on fuel vaporization is so small that α_{E0} and α_{E20} nearly coincide and must be plotted in different colors.

Figure 6-1
The PME-A Index for PFI Vehicles



This is an empirical result that does not require interpretation, but we note that it is directionally consistent with the longer period of time that atomized fuel is resident in a PFI engine and subject to vaporization before combustion begins. Figure 6-2 plots the α coefficients in PME as a function of ethanol content for both SIDI and PFI vehicles. For PFI, the α line between E0→E10 is nearly flat, while it steepens after E10 and becomes nearly parallel to the conjectural extension of the α line for SIDI vehicles. This suggests that the cooling effect of ethanol through E10 is offset to some extent by the longer residence time and vaporization period in PFI engines.

Figure 6-2
Impact of Ethanol Content on the α Term in $1/VP\alpha$



6.2 Performance of the PME-A Index for PFI Vehicles

Following estimation of the coefficient values, the PME-A index for SIDI vehicles was evaluated for completeness by examining the LA92 Phase I PM emission residuals from the model versus a series of fuel variables. The objective was to determine whether the index fit all fuels and whether other fuel properties would improve the index. This was done using the EPAAct dataset from which the index was estimated. There are no other test programs in which the EPAAct fuels were used and no recent, large test programs involving PFI vehicles.

The LA92 Phase I PM emission residuals for one E10 fuel (Fuel 11) stood off the PME-A by a statistically significant value ($p=0.0002$). With 27 fuels, one fuel might to exceed the $p=0.01$ threshold by chance alone in about one of four studies. Given this and with just one data point, there is no basis to investigate possible causes with the available data. The emission averages for two other fuels—Fuel 10 at E10 and Fuel 25 at E20—are offset from the PME-A line but by amounts that do not reach the $p=0.01$ level. Further analysis of the three fuels *might* shed additional light on the mechanism of PM formation from fuels and its representation in PME.

The LA92 Phase I PM emission residuals were tested against the same range of bulk fuel properties to see if another variable might improve PME-A performance. The set of fuel variables that determine PM emissions from vehicles has been a subject of some debate. The EPAAct analysis reported in EPAAct 2013a examined the bulk fuel properties used in the experiment design and identified aromatics and ethanol content and T50 and T90 points on the distillation curve as significant predictors for LA92 Phase I PM emissions. Aromatics content and T90 are widely recognized indicators of a fuel's sooting potential, and it is accepted that the presence of ethanol tends to increase emissions even though the ethanol

molecule produces little or no soot on its own. The role of T50—a measure of mid-range volatility—in PM formation is less-well understood. The work in Butler 2015 re-examined the EPAAct dataset using the Honda PMI and found that ethanol content and T50 were still significant predictors of PM emissions.

Table 6-3 shows the subset of bulk fuel properties that came close to statistical significance in both SIDI and PFI vehicles. While RVP and the related T05 distillation point were found to be possible predictors of the emissions offsets of two fuels in E-94-2 (see Section 4.2.1), neither variable comes close to significance in the EPAAct dataset. In fact, the PME-A index performs well in both EPAAct groups of RVP 7 and 10 psi fuels.

Table 6-3
Statistical Significance of Other Fuel Properties
in the Phase I PM Residuals for PME-A for PFI Vehicles

Fuel Property	SIDI Vehicles (E-94-2)	PFI Vehicles (EPAAct)		
		E0 Fuels	E0-E10	E0-E20
RVP	p < 0.001	p = 0.35	p = 0.22	p = 0.18
T05	p < 0.003	p = 0.16	p = 0.41	p = 0.28
T50	—	p = 0.025	p = 0.048	p = 0.028
T60	p = 0.07	p = 0.015	p = 0.048	p = 0.026
T70	p = 0.07	p = 0.028	p = 0.017	p = 0.06
T80	—	p = 0.08	p = 0.019	p = 0.12
E200F	Not tested	p = 0.032	p = 0.088	p = 0.10

Given the past interest in mid-range volatility, T50 and nearby distillation points were closely examined throughout the work. For SIDI vehicles, the T60 and T70 points approached the conventional threshold for statistical significance (p=0.05) but fell short of the p=0.01 threshold used in this work. For PFI vehicles, a range of distillation points from T50 through T80 and E200F¹¹ come close to, or achieve, the conventional threshold for significance. The significance of variables differs by fuel group as does the “best” choice of variable.

The most reliable test is that made in the E0 fuels group. The addition of ethanol influences the T50 distillation point and, as the ethanol content increases, it becomes difficult (in E15 fuels) or impossible (in E20 fuels) to independently control T50; this complication is not

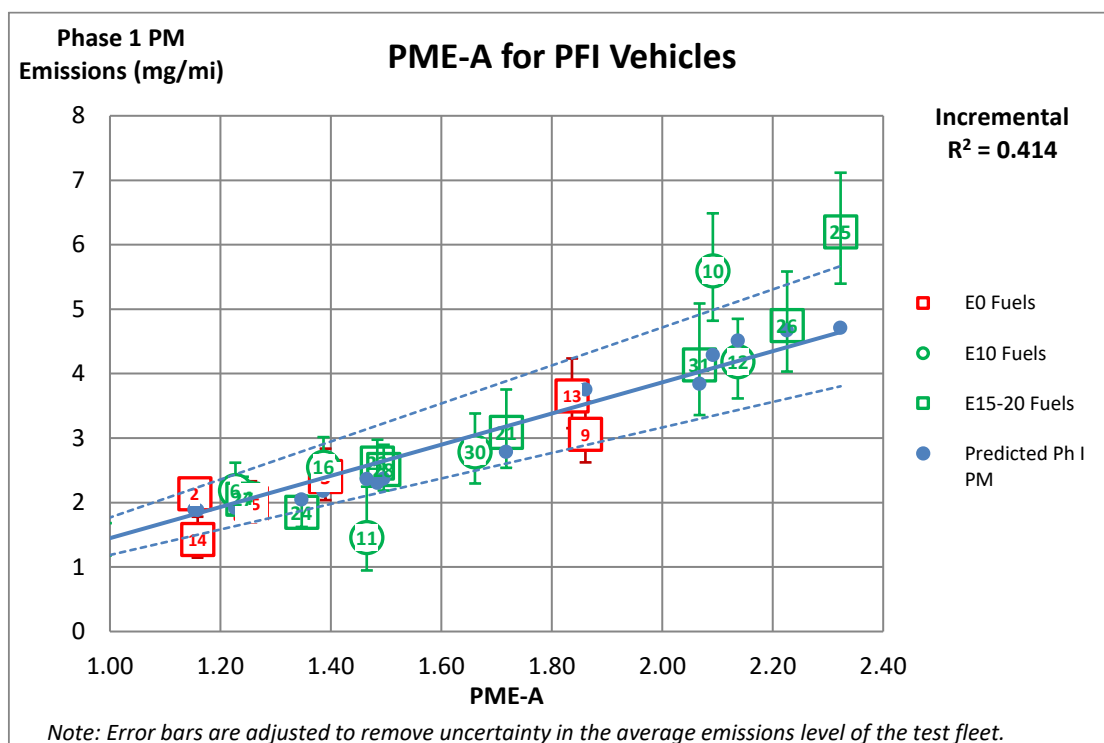
¹¹ The fuel fraction that evaporates at temperatures ≤ 200°F.

present for E0 fuels. As the table shows, T50, T60, and T70 reach the conventional level for significance, with T60 being slightly “better.”

From a statistical perspective, there may be merit in the hypothesis that mid-range volatility plays a role in PM emissions from vehicles. However, none of the distillation points or other fuel properties reach the $p=0.01$ level used throughout this work. Thus, the PME-A index for PFI vehicles is deemed to be a complete in the sense that no other fuel property can be shown to add explanatory power for PM emissions with the currently available data.

Figure 6-3 shows the performance of PME-A as a predictor of LA92 Phase 1 PM emissions in the EPAAct dataset. The overall trend line is plotted in blue with dotted lines for its 95% confidence interval. Average PM emissions for each fuel are plotted in red and green with different symbols used to distinguish the four level of ethanol (E0, E10, E15, and E20). As explained in Section 4.2.1, the error bars have been adjusted to better reflect the relationship of the fuel data points to the overall PME-A trend line.

Figure 6-3
Comparison of Actual versus Predicted Emissions for PFI Vehicles



The linearity of LA92 Phase I PM emissions with PME-A is easily seen and the linearity holds for both E0 fuels and ones containing ethanol. Three fuels—Fuels 10, 11, and 25—stand off the PME-A line more than the others and might hold some additional insight on PM formation in PFI vehicles. The scatter of fuels around the PME-A is significantly

reduced compared to the corresponding chart for the Honda PMI in CRC RW-107 (reproduced as Figure 6-4¹²).

Figure 6-4
The Relationship of LA92 Phase I PM Emissions to the Honda PMI

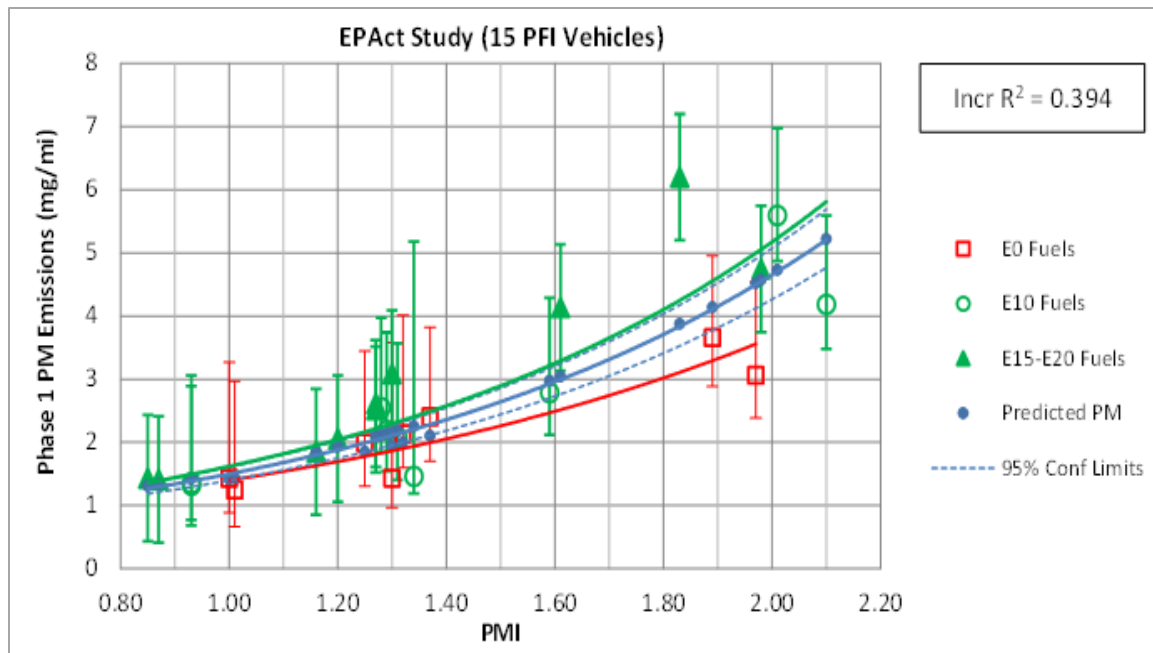


Table 6-4 summarizes the several measures of index performance; see Section 4.2.1 for their definition. PME-A is a clear improvement over the Honda PMI in the Incremental R^2 and the RMS and MAE error statistics. The ethanol bias of the Honda PMI is eliminated at all three ethanol content levels; the result for E20 fuels is strongly influenced by Fuel 25 and may be fuel-specific rather than an indicator of ethanol bias itself.

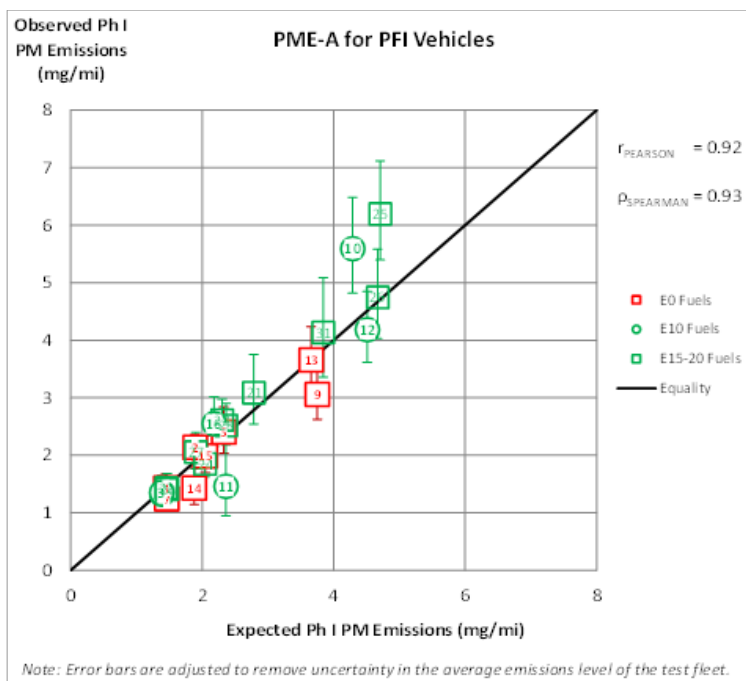
PME-A also performs well in ranking the fuels for emissions as seen in the table and in Figure 6-5. The Pearson r and Spearman ρ correlation coefficients are both high; the Spearman ρ (indicative for ranking success) achieves the same high value as PME-A and PME-B for SIDI vehicles. Some ranking errors are made. For example, Fuel 13 is ranked lower for PM than Fuel 9 and Fuel 10 is ranked lower than Fuel 12. But such errors cannot be avoided for fuels that are close in emissions. PME-A would be suitable for guiding the tradeoff between composition and PM emissions for research purposes, even if its form is too complex for use in fuel blending.

¹² Note that the error bars in the chart are based on the usual calculation and have not been adjusted as in the preceding figure.

Table 6-4
Performance Measures for the PME-A Index for PFI Vehicles

	PME-A This Study		Honda PMI* RW-107
Incremental R ²	0.414		0.394
r _{PEARSON}	0.92		n/a
ρ _{SPEARMAN}	0.93		n/a
Error Metric			
RMS Error	7%		24%
MAE	11%		60%
EtOH Bias	Percent	Prob> t	Percent
E10	6%	p = 0.93	n/a
E15	12%	p = 0.19	n/a
E20	13%	p = 0.07	n/a
* After PMI is linearized by an empirically fit exponent.			

Figure 6-5
Ranking of EPAct Fuels for PM Emissions using PME-A for PFI



6.3 Discussion

The performance analysis demonstrates that PME-A is an effective indicator of LA92 Phase I PM emissions from PFI vehicles and is without bias with respect to ethanol content over the range E0 to E20. It can be used to compare finished gasolines of RVP 7 psi and 10 psi for use in PFI vehicles. Although the EPAAct dataset was demonstrated only for the two specific RVP levels, it is likely that PME-A can be used to compare fuels with a range of RVP levels in between. It is also complete in the sense that no other fuel property can be shown to add explanatory power for PM emissions with the currently available data.

Its use is subject to the caveat that it must be restricted to fuels of RVP 7~10, although the performance analysis says that can include cross comparisons between fuels at 7 and 10 psi. It cannot be used in its current form to guide blending of ethanol into BOBs in a manner sensitive to achieving PM emission reductions because it does not accurately indicate the BOB's emissions potential.

CRC plans further work to acquire new data on PM emissions from PFI vehicles. The planned datasets will provide some degree of independent validation, but they will have test fleets of only three PFI vehicles. Further development of the PME index for PFI vehicles may depend upon the conduct of testing programs not currently envisioned.

7. CORRELATION INDICES FOR PM BASED ON PME

A simplified PM index that is based on common bulk fuel properties or on a simplified hydrocarbon speciation may be of interest. In an attempt to provide for this need, four different, correlation-based PM indices, previously examined in RW-107, were re-estimated to predict the PME-A values, rather than the Honda PMI values used originally to define them. A discussion of these indices can be found in Section 3 of CRC RW-107 (2019). The re-estimation was done using the fuels of the CRC E-94-2 and EPAAct studies, which were combined to increase sample size.¹³

The eight fuels from E-94-2 are too few in number to yield reliable indices; for example, the PEI index has five coefficients. By adding the 27 EPAAct fuels, not only is the sample size increased, but also the range of fuel properties is greatly expanded. Splash-blended fuels from E-94-3 and E-129 were excluded because PME does not accurately reflect the PM emissions from the fuels.

The updated correlation indices are given in Table 7-1 below. The original formulation is given first for each of the indices. Then, the index is given in two ways: as updated from the combined dataset; and as updated when the leading energy content term from PME is included. Coefficient values are given with their standard errors below. Statistical significance is indicated with **bold** for coefficients achieving at least $p \leq 0.05$, with a superscript giving the level of significance as explained in the table.

Overall, the results presented in the table show low statistical correlation among the indices with PME. Only PEI has an acceptably high $R^2 = 0.78$; the other three indices have such low R^2 value that they would not be useful in fuel blending. PEI is based on a PIONA speciation of the aromatic hydrocarbon content, which sets it apart from the others, which are based only on bulk fuel properties. While PEI fares the best in this evaluation, it is not possible to estimate statistically significant values for all of its coefficients. Estimation is improved in the second form (with the energy adjustment term), but coefficients could not be estimated for the C8 and C10 terms.

For the indices based on bulk fuel properties, the estimated coefficients achieve significance in only one case, although those for the PASCE index come close to $p=0.05$. An index based on bulk fuel properties relies upon the fuels used in its estimation having the same correlations among fuel properties that will exist in the fuels to which it is applied. The EPAAct fuels were designed to fill an orthogonal design involving aromatics and ethanol contents, T50 and T90 distillation points, and RVP. Achieving orthogonality necessarily

¹³ The datasets were analyzed separately in development of PME because the emissions response differed between SIDI and PFI vehicles. That difference is not relevant here and there is no impediment to combining the datasets.

implies breaking the usual correlations among those five properties. Thus, the EPAAct dataset may not be a useful basis for estimating indices that rely on bulk properties.

The outcome for PEI is undoubtedly a result of how high and low PM fuels were created by the specialty blender for the two studies. Specifically:

- For E-94-2, the fuels have only one degree of freedom in how PM potential was varied that likely involved a single, heavy blendstock that would have carried compounds in the C11 and higher groups. In such a case, the fuels could contribute to the final PEI term for the C11 and higher group, but not the other terms.
- For EPAAct, the fuels have two degrees of freedom in that both aromatics content and the T90 boiling point were varied independently in the experiment design. These fuels can contribute to the final term for the C11 and higher although the EPAAct DHAs show only a few C12 compounds and no C13 or higher compounds.

Variation of aromatics content likely involved changes in the C7 to C10 groups, but the variations may have been concentrated in some of the groups, and not in the others, as a result of the blender's choice for a high aromatics blendstock(s). Such gaps in the variation of aromatic hydrocarbons, if present, would make it impossible to estimate coefficients for some CN groups (such as C8 and C10).

Overall, the outcome falls well short of the goal to provide fuel blenders with a simplified PM index. Further, the outcome illustrates the importance of basing the indices on a dataset of fuels similar to the commercial gasolines that fuel blenders would create. The needed dataset can be described as a sample of commercial gasolines for which DHAs are available along with a range of bulk fuel properties. The fuels should cover the range of aromatics and ethanol contents found in recent U.S. markets, or a somewhat wider range, to assure that sufficient variation exists for the two variables. A sample of about 30 well-chosen fuels should suffice to develop simplified indices.

Table 7-1
Correlation-based PM Indices Updated for PME-A

Index	Reference	Mathematical Form	Goodness of Fit
PEI	Chapman (2018)	$\text{PMI} = \text{C7}_{\text{AROM}} + 2.5 \cdot \text{C8}_{\text{AROM}} + 5.8 \cdot \text{C9}_{\text{AROM}} + 4.8 \cdot \text{C10}_{\text{AROM}} + 35.3 \cdot (\text{C11}_{\text{AROM}} + \text{C12}_{\text{AROM}} + \text{C13}_{\text{AROM}})$	
		$\text{PME-A} = \left[\begin{array}{cccc} 1.7 \cdot \text{C7}_{\text{AROM}} & + 0.28 \cdot \text{C8}_{\text{AROM}} & + 4.2^* \cdot \text{C9}_{\text{AROM}} & + 0.0 \cdot \text{C10}_{\text{AROM}} \\ \pm 1.6 & \pm 1.9 & \pm 1.1 & \text{n/a} \end{array} + 38.6^{\ddagger} \cdot (\text{C11}_{\text{AROM}} + \text{C12}_{\text{AROM}} + \text{C13}_{\text{AROM}} + \text{C14}_{\text{AROM}}) \right] / 100$ ± 3.9	R ² =0.78
		$\text{PME-A} = \frac{43.4}{\text{LHV}} \cdot \left[\begin{array}{cccc} 1.89^* \cdot \text{C7}_{\text{AROM}} & + 0.0 \cdot \text{C8}_{\text{AROM}} & + 3.75^* \cdot \text{C9}_{\text{AROM}} & + 0.0 \cdot \text{C10}_{\text{AROM}} \\ \pm 0.52 & \text{n/a} & \pm 0.91 & \text{n/a} \end{array} + 38.4^{\ddagger} \cdot (\text{C11}_{\text{AROM}} + \text{C12}_{\text{AROM}} + \text{C13}_{\text{AROM}} + \text{C14}_{\text{AROM}}) \right] / 100$ ± 3.6	R ² =0.78
PASCE	Chapman (2016)	$\text{PMI} = 9.37 + 0.517 \cdot \text{C/H} - 0.11994 \cdot \text{E170}$	
		$\text{PME-A} = \begin{array}{ccc} 2.48 & + 0.31 \cdot \text{C/H} & - 3.70 \cdot \text{E170} \\ \pm 1.92 & \pm 0.17 & \pm 1.89 \end{array}$	R ² =0.17
		$\text{PME-A} = \frac{43.4}{\text{LHV}} \cdot \left[\begin{array}{ccc} 2.48 & + 0.30 \cdot \text{C/H} & - 3.62 \cdot \text{E170} \\ \pm 1.86 & \pm 0.16 & \pm 1.83 \end{array} \right]$	R ² =0.16

Index	Reference	Mathematical Form	Goodness of Fit
E150	Moriya (2016)	PMI = 7.8511 - 0.0757 · E150	
		PME-A = 2.41* -1.78 · E150 ±0.96 ±1.15	R ² =0.06
		PME-A = $\frac{43.4}{LHV} \cdot [2.24 -1.57 \cdot E150]$ ±0.93 ±1.10	R ² =0.06
E130-170	Moriya (2016)	PMI = 9.9241 - 0.0324 · E130 - 0.0647 · E170	
		PME-A = 3.15 -1.20 · E130 -1.41 · E170 ±2.08 ±1.47 ±1.47	R ² =0.10
		PME-A = $\frac{43.4}{LHV} \cdot [3.21 -0.92 \cdot E130 -1.74 \cdot E170]$ ±2.04 ±1.42 ±2.93	R ² =0.08
Coefficients that achieve statistical significance (p≤0.05) are highlighted in Bold . A superscript symbol gives the level of significant as follows: * p ≤ 0.05 but not ≤ 0.01 † p ≤ 0.01 but not ≤ 0.001 ‡ p ≤ 0.001 or better Coefficients not marked fail to achieve p ≤ 0.05			

8. SUMMARY AND DISCUSSION

8.1 Summary

This report has presented a “new technology” PM index termed PME that is applicable to the fuels that are available in the U.S. market today and used in both SIDI and PFI vehicles. Table ES-1, reproduced below as Table 8-1, summarizes the mathematical form and the empirical coefficients needed to apply PME to DHAs for fuels in place of the Honda PMI.

Table 8-1
The PME Formulation

$\text{PME} = \left(\frac{43.4}{\text{LHV}} \right) \cdot \left[\textcolor{green}{N_{TECH}} \cdot \sum_i \frac{\text{wt}\%_i \cdot \textcolor{green}{yTerm_i}}{VP_i^{\alpha=f(\text{EtOH})}} \right]^\beta$ $\alpha = \{ \alpha_{\text{E0}}, \alpha_{\text{E10}}, \alpha_{\text{E20}} \}$ $f(\text{EtOH}) = \alpha_{\text{E0}} + \Delta\alpha \cdot \text{EtOH}_{\text{VOL}\%}$ LHV = Lower Heating Value							
$yTerm_i = (\text{C}+\text{O}-1) \cdot (1 + 1.7 \cdot \text{DBE}_{\text{NON}} + 5.6 \cdot \text{ArRing}_{\text{FIRST}} + 5.1 \cdot \text{ArRings}_{\text{ADD}})$							
Engine Technology	DHA Type	Designation	N _{TECH}	α _{E0}	α _{E10}	α _{E20}	β
SIDI	ASTM	PME-A	0.00597	0.456	0.443	—	1.17
	SSI	PME-B	0.00597	0.456	0.443	—	1.00
PFI	ASTM	PME-A	0.0109	0.564	0.558	0.531	1.17
	SSI	PME-B	No data is presently available				
Note: Green font denotes empirically estimated parameters.							

The Honda PMI has supported a large body of research on the link between fuels and PM emissions from motor vehicles over the past decade. The work performed for this project has improved upon the Honda PMI in the following ways:

- The 1+DBE numerator in the Honda Eq. has been replaced by an empirical formula called the “yTerm” that estimates the chemical sooting potential of individual hydrocarbons based on the YSI Version 2 database.
- The VP term in the denominator has been modified to adopt an exponent α that governs the relative contributions of heavy versus light hydrocarbons to PM emissions in a manner that varies by engine technology (SIDI versus PFI).

In addition, the work has extended the range of fuel effects that it represents. The Honda PMI accounts only for the benefit of ethanol blending—the dilution of gasoline hydrocarbons by an oxygenate that produces little/no soot itself. The PME formulation extends this in two ways:

- The α coefficient is made a function of ethanol content to account for the cooling effect caused by ethanol's high heat of vaporization and tendency to form near-azeotropes, which tends to increase the fractions of heavier hydrocarbons that are less completely volatilized and, thus, the yield of soot.
- A term has been included to adjust PME for differences in energy content in fuels. Fuels oxygenated with ethanol and a number of other compounds have lower energy contents on a weight basis (per kg) than an E0 or “neat” gasoline. Therefore, a larger quantity of the blended fuel must be burned to power a vehicle over the drive cycle used to measure PM emissions.

Additional work is needed with independent datasets to validate PME's performance across a wider range of vehicles and fuel. At present, the chief limitation is that its performance has been demonstrated only for finished fuels that have been blended to an RVP specification of 7 psi for SIDI vehicles and 7~10 psi for PFI vehicles. With respect to ethanol content, its performance has been demonstrated for E0 and E10 fuels in SIDI vehicles and for E0, E10, E15 and E20 fuels in PFI vehicles.

The PME formulation is considered most applicable to research work as it requires the conduct of a DHA to determine hydrocarbon composition. Simplified indices will be needed for fuel blending and other purposes where the expense of a DHA is not warranted, but the effort to develop such indices was unsuccessful in this study.

8.2 Discussion

The PME formulation provides a more complete indication of the PM potential of fuels and one that can differ substantially from that of the Honda PMI. Appendix C tabulates the PME values for the experimental fuels used in this work. Authors of prior research that used the Honda PMI should consider whether conclusions on PM emissions and fuels could be affected. This is mostly likely when emissions analysis was done using PMI (or a similar form) as a predictor for PM emissions in work that was intended to identify other factors influencing PM emissions. Examples include Butler 2015 and St. John 2019. The use of PME instead of PMI should increase the variance associated with the index and leave less to be associated with other variables, which may to different conclusions regarding their contributions and statistical significance.

For the primary datasets used in this work, past analysis and conclusions would not be changed by the adoption of PME in place of PMI. Specifically:

- The analysis of the EPAAct data reported in EPAAct 2013a did not involve the Honda PMI, which had not been published when the EPAAct testing program began. Because PMI was not used, the original statistical analysis is not changed nor should conclusions that were drawn from it.
- The CRC E-94-2 study examined PM emissions from SIDI vehicles in an experiment design where the Honda PMI determined the fuels' propensities to soot. The main conclusion should be stated: *ethanol increases PM emissions from SIDI vehicles over and above the level that would be expected from an E0 fuel of the same PMI*. This remains correct today because the conclusion regarding emission increases was contingent upon equal PMIs.

However, the perspective has changed given the new PME index. We would now say that PM emissions from SIDI vehicles are expected to be comparable on any set of fuels that have the same PME index, whether they are non-oxygenated fuels or fuels oxygenated with ethanol.

- The CRC E-94-3 study compared PM emissions from the E0 fuels in E-94-2 to emissions from E10 fuels created from them by splash blending. The main conclusion was that, on average, PM emissions were higher in the splash-blended E10 fuels than in the E0 fuels. This is based on observed emissions without reference to PMI and remains correct today.

While additional work is needed to validate and, possibly, improve on PME, its primary limitation at present is that it does not accurately predict the increase in PM emissions from splash-blended fuels (as observed in E-94-3). This precludes its use to guide ethanol blending into BOBs to achieve desired reductions in PM emissions.

Finally, the effort to create simplified PM indices for fuel blending was unsuccessful due to the nature of the experimental fuels in the CRC and EPAAct studies. This task needs a dataset of fuels similar to the commercial gasolines that fuel blenders would create, not datasets from orthogonal experiment designs that may change or break the correlations of some fuel properties.

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APPENDIX A

MASTER LIST OF HYDROCARBON COMPOUNDS

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
Propene	Olefin	3	3	1	1	1	0	0	5.4	225.1	16,957		
Propane	Alkane	3	3	0	2	0	0	0	2.0	231.2	14,398		
i-Butane	Alkane	4	4	0	3	0	0	0	3.0	261.4	6,655		
Isobutene	Olefin	4	4	1	2	1	0	0	8.1	266.2	5,928		
Butene-1	Olefin	4	4	1	2	1	0	0	8.1	271.4	5,237		
n-Butane	Alkane	4	4	0	3	0	0	0	3.0	272.6	5,091		
t-Butene-2	Olefin	4	4	1	2	1	0	0	8.1	274.0	4,926		
c-Butene-2	Olefin	4	4	1	2	1	0	0	8.1	276.8	4,612		
2,2-Dimethylpropane	Alkane	5	5	0	4	0	0	0	4.0	280.3	4,250		
3-Methylbutene-1	Olefin	5	5	1	3	1	0	0	10.8	293.3	3,158		
i-Pentane	Alkane	5	5	0	4	0	0	0	4.0	303.2	2,523		
2-Methylbutene-1	Olefin	5	5	1	3	1	0	0	10.8	304.4	2,456		
2-Methyl-1,3-Butadiene	Olefin	5	5	2	2	2	0	0	17.6	307.2	2,301		
2-methyl-2-butene	Olefin	5	5	1	3	1	0	0	10.8	308.1	2,255	43.5	2.0
cis 2-pentene	Olefin	5	5	1	3	1	0	0	10.8	308.1	2,255	39.8	2.1
n-pentane	Alkane	5	5	0	4	0	0	0	4.0	308.3	2,245	24.6	2.4
Pentene-1	Olefin	5	5	1	3	1	0	0	10.8	309.1	2,205		
Cyclopropane, ethyl-	Naphthene	5	5	1	5	0	1	0	10.8	309.3	2,199		
t-Pentene-2	Olefin	5	5	1	3	1	0	0	10.8	310.1	2,156		
cyclopentadiene	Naphtheno-Olefin	5	5	3	3	2	1	0	24.4	314.0	1,978		
3,3-dimethyl-1-butene	Olefin	6	6	1	4	1	0	0	13.5	314.4	1,962	53.1	2.0
1,3-Cyclopentadiene	Naphtheno-Olefin	5	5	3	3	2	1	0	24.4	317.3	1,839		
1t,3-Pentadiene	Olefin	5	5	2	2	2	0	0	17.6	317.3	1,839		
1c,3-Pentadiene	Olefin	5	5	2	2	2	0	0	17.6	317.3	1,837		
cyclopentene	Naphtheno-Olefin	5	5	2	4	1	1	0	17.6	317.4	1,835	80.5	2.1
2,2-dimethylbutane	Alkane	6	6	0	5	0	0	0	5.0	321.6	1,671	43.4	2.0
cyclopentane	Naphthene	5	5	1	5	0	1	0	10.8	322.5	1,637	39.4	2.1
4-Methylpentene-1	Olefin	6	6	1	4	1	0	0	13.5	326.9	1,484		
ethanol	Alkane	2	3	0	2	0	0	0	2.0	351.6	1,475	10.3	2.9

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
2,3-dimethyl-1-butene	Olefin	6	6	1	4	1	0	0	13.5	328.8	1,423	53.4	2.0
3-methyl-1-pentene	Olefin	6	6	1	4	1	0	0	13.5	329.4	1,404	45.1	2.0
cis 4-methyl-2-pentene	Olefin	6	6	1	4	1	0	0	13.5	330.2	1,379	54.1	2.0
4-methyl-1-pentene	Olefin	6	6	1	4	1	0	0	13.5	331.5	1,338	50.2	2.0
2,3-dimethylbutane	Alkane	6	6	0	5	0	0	0	5.0	331.9	1,328	44.0	2.0
2-methylpentane	Alkane	6	6	0	5	0	0	0	5.0	332.8	1,302	36.7	2.1
1-hexene	Olefin	6	6	1	4	1	0	0	13.5	335.1	1,234	42.4	2.0
2-ethyl-1-butene	Olefin	6	6	1	4	1	0	0	13.5	335.1	1,234	45.6	2.0
2-methyl-1-pentene	Olefin	6	6	1	4	1	0	0	13.5	335.1	1,234	42.9	2.0
3-methylpentane	Alkane	6	6	0	5	0	0	0	5.0	335.8	1,215	38.2	2.1
3-methyl-2-pentene	Olefin	6	6	1	4	1	0	0	13.5	337.7	1,164	53.7	2.0
3-Methyl-t-pentene-2	Olefin	6	6	1	4	1	0	0	13.5	337.7	1,164		
3-Methylcyclopentene	Naphtheno-Olefin	6	6	2	5	1	1	0	22.0	338.0	1,157		
C6_Naphtheno-Olefins(2)	Naphtheno-Olefin	6	6	2	5	1	1	0	22.0	338.0	1,157		
C6_Naphtheno-Olefins(3)	Naphtheno-Olefin	6	6	2	5	1	1	0	22.0	338.0	1,157		
methanol	Alkane	1	2	0	1	0	0	0	1.0	337.8	1,154	6.6	3.0
trans 3-hexene	Olefin	6	6	1	4	1	0	0	13.5	338.7	1,139	47.2	2.0
4-methylcyclopentene	Naphtheno-Olefin	6	6	2	5	1	1	0	22.0	338.9	1,136		
4-Methyl-t-pentene-2	Olefin	6	6	1	4	1	0	0	13.5	340.4	1,098		
2-methyl-2-pentene	Olefin	6	6	1	4	1	0	0	13.5	340.4	1,096	53.6	2.0
c-Hexene-3	Olefin	6	6	1	4	1	0	0	13.5	340.8	1,087		
cis 2-hexene	Olefin	6	6	1	4	1	0	0	13.5	340.8	1,087	44.7	2.0
3-Methyl-c-pentene-2	Olefin	6	6	1	4	1	0	0	13.5	340.8	1,087		
trans 2-hexene	Olefin	6	6	1	4	1	0	0	13.5	341.0	1,082	45.8	2.0
Methyl-t-butyl ether	Alkane	5	7	0	5	0	0	0	6.0	328.2	1,075		
n-hexane	Alkane	6	6	0	5	0	0	0	5.0	341.8	1,063	30.4	2.3
methylcyclopentane	Naphthene	6	6	1	6	0	1	0	13.5	345.0	992	50.3	2.0
5-methyl-1,3cyclopentadiene	Naphtheno-Olefin	6	6	3	4	2	1	0	30.5	345.7	974		
C6-Diolefin-1	Olefin	6	6	2	3	2	0	0	22.0	348.6	913		
4-Methyl-1,3-pentadiene	Olefin	6	6	2	3	2	0	0	22.0	349.6	893		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
2,2-dimethylpentane	Alkane	7	7	0	6	0	0	0	6.0	351.1	865	47.4	2.0
1,4-Pentadiene, 3,3-dimethyl-	Olefin	7	7	2	4	2	0	0	26.4	351.3	862		
1-methyl-1-cyclopentene	Naphtheno-Olefin	6	6	2	5	1	1	0	22.0	351.6	856	97.7	5.9
2,3,3-trimethyl-1-butene	Olefin	7	7	1	5	1	0	0	16.2	352.5	839	72.8	2.2
3,3-Dimethylpentene-1	Olefin	7	7	1	5	1	0	0	16.2	352.8	833		
3,4-Dimethylpentene-1	Olefin	7	7	1	5	1	0	0	16.2	352.8	833		
benzene	Aromatic	6	6	4	3	0	0	1	33.0	353.2	824	100.3	5.8
2,4-dimethylpentane	Alkane	7	7	0	6	0	0	0	6.0	353.6	817	49.6	2.0
cyclohexane	Naphthene	6	6	1	6	0	1	0	13.5	353.8	813	42.7	2.0
2,2,3-trimethylbutane	Alkane	7	7	0	6	0	0	0	6.0	354.8	795	55.3	2.0
tert-butyl ethyl ether	Alkane	6	7	0	6	0	0	0	6.0	346.0	777	37.9	2.1
2-Pentene, 2,4-dimethyl-	Olefin	7	7	1	5	1	0	0	16.2	356.5	765		
1-Pentene, 2,3-dimethyl-	Olefin	7	7	1	5	1	0	0	16.2	358.2	737		
2,4-Dimethylpentene-1	Olefin	7	7	1	5	1	0	0	16.2	358.3	737		
2-Ethyl-3-methylbutene-1	Olefin	7	7	1	5	1	0	0	16.2	358.2	737		
5-Methylhexene-1	Olefin	7	7	1	5	1	0	0	16.2	358.4	733		
3-Ethylpentene-1	Olefin	7	7	1	5	1	0	0	16.2	358.5	732		
3-Methylhexene-1	Olefin	7	7	1	5	1	0	0	16.2	358.5	732		
4-methyl-1-hexene	Olefin	7	7	1	5	1	0	0	16.2	358.5	732	55.8	2.0
cyclohexene	Naphtheno-Olefin	6	6	2	5	1	1	0	22.0	358.7	728	62.2	2.0
2-Methyl-t-hexene-3	Olefin	7	7	1	5	1	0	0	16.2	359.1	723		
3,3-dimethylpentane	Alkane	7	7	0	6	0	0	0	6.0	359.2	720	47.7	2.0
1,4-Hexadiene, 2-methyl-	Olefin	7	7	2	4	2	0	0	26.4	360.3	704		
C7_Mono-Naphthenes(1)	Naphthene	7	7	1	7	0	1	0	16.2	360.6	698		
1,1-Dimethylcyclopentane	Naphthene	7	7	1	7	0	1	0	16.2	360.6	698		
Cyclopentene, 4,4-dimethyl-	Naphtheno-Olefin	7	7	2	6	1	1	0	26.4	360.9	695		
Benzene	Aromatic	6	6	4	3	0	0	1	33.0	361.1	691		
(Z)-4-Methyl-2-hexene	Olefin	7	7	1	5	1	0	0	16.2	361.5	684		
2-Hexene, 4-methyl-, (E)-	Olefin	7	7	1	5	1	0	0	16.2	361.5	684		
2-Methyl-c-hexene-3	Olefin	7	7	1	5	1	0	0	16.2	361.5	684		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
4-Methyl-t/c-hexene-2	Olefin	7	7	1	5	1	0	0	16.2	361.5	684	49.4	2.0
5-Methyl-c-hexene-2	Olefin	7	7	1	5	1	0	0	16.2	361.5	684		
2,3-dimethylpentane	Alkane	7	7	0	6	0	0	0	6.0	362.9	663		
2-Pentene, 3,4-dimethyl-, (Z)-	Olefin	7	7	1	5	1	0	0	16.2	363.2	660		
2-Pentene, 3,4-dimethyl-, (E)-	Olefin	7	7	1	5	1	0	0	16.2	363.2	660	42.4	2.0
2-methylhexane	Alkane	7	7	0	6	0	0	0	6.0	363.2	658		
5-Methyl-t-hexene-2	Olefin	7	7	1	5	1	0	0	16.2	363.3	658		
2,3-dimethyl-2-pentene	Olefin	7	7	1	5	1	0	0	16.2	363.5	655		
3-Methyl-t-hexene-2	Olefin	7	7	1	5	1	0	0	16.2	363.6	653	43.0	2.0
1,5-Heptadiene	Olefin	7	7	2	4	2	0	0	26.4	363.6	652		
t-Heptene-2	Olefin	7	7	1	5	1	0	0	16.2	363.7	651		
3-methylhexane	Alkane	7	7	0	6	0	0	0	6.0	363.8	649		
1c,3-Dimethylcyclopentane	Naphthene	7	7	1	7	0	1	0	16.2	363.9	648	49.1	2.0
2-Methylhexene-1	Olefin	7	7	1	5	1	0	0	16.2	364.0	647		
2-methyl-1-hexene	Olefin	7	7	1	5	1	0	0	16.2	364.0	647		
1t,3-Dimethylcyclopentane	Naphthene	7	7	1	7	0	1	0	16.2	364.8	635		
2-Ethylpentene-1	Olefin	7	7	1	5	1	0	0	16.2	364.9	634	365.0	632
1t,2-Dimethylcyclopentane	Naphthene	7	7	1	7	0	1	0	16.2	365.0	632		
C7 - Iso-Olefin - 2	Olefin	7	7	1	5	1	0	0	16.2	365.2	630		
3-Ethylpentane	Alkane	7	7	0	6	0	0	0	6.0	365.5	626		
C7 - MonoNaph - 1	Naphthene	7	7	1	7	0	1	0	16.2	366.2	616	59.8	2.0
3-ethyl-2-pentene	Olefin	7	7	1	5	1	0	0	16.2	366.5	611		
3-Methyl-c-hexene-3	Olefin	7	7	1	5	1	0	0	16.2	366.5	611		
3-Methyl-t-hexene-3	Olefin	7	7	1	5	1	0	0	16.2	366.6	610		
1-heptene	Olefin	7	7	1	5	1	0	0	16.2	366.7	608	48.4	2.0
c-Heptene-3	Olefin	7	7	1	5	1	0	0	16.2	367.5	598		
2-Methyl-2-hexene	Olefin	7	7	1	5	1	0	0	16.2	368.5	584		
c-Heptene-3	Olefin	7	7	1	5	1	0	0	16.2	368.7	582		
trans 3-heptene	Olefin	7	7	1	5	1	0	0	16.2	368.8	580	53.5	2.0
3,5-Dimethylcyclopentene	Naphtheno-Olefin	7	7	2	6	1	1	0	26.4	369.3	574		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
1c,2-Dimethylcyclopentane	Naphthene	7	7	1	7	0	1	0	16.2	370.4	561	16.2	2.7
1-propanol	Alkane	3	4	0	3	0	0	0	3.0	370.3	561		
3-Methyl-c-hexene-2	Olefin	7	7	1	5	1	0	0	16.2	370.4	560		
3-Ethylcyclopentene	Naphtheno-Olefin	7	7	2	6	1	1	0	26.4	371.0	553	61.7	2.0
2,2,4-trimethylpentane	Alkane	8	8	0	7	0	0	0	7.0	371.1	551		
c-Heptene-2	Olefin	7	7	1	5	1	0	0	16.2	371.5	546		
n-heptane	Alkane	7	7	0	6	0	0	0	6.0	371.5	546	36.0	2.2
2-Heptene	Olefin	7	7	1	5	1	0	0	16.2	371.6	545		
Cyclopropane, butyl-	Naphthene	7	7	1	7	0	1	0	16.2	372.3	537		
2-butanol	Alkane	4	5	0	4	0	0	0	4.0	372.0	532	24.8	2.4
methylcyclohexane	Naphthene	7	7	1	7	0	1	0	16.2	374.0	516		
1-Pentene, 2,4,4-trimethyl-	Olefin	8	8	1	6	1	0	0	18.9	374.6	509		
2,4,4-trimethyl-1-pentene	Olefin	8	8	1	6	1	0	0	18.9	375.0	505	68.5	2.1
1,4-Pentadiene, 2,3,4-trimethyl	Olefin	8	8	2	5	2	0	0	30.8	375.1	503		
Cyclopentene, 1,5-dimethyl-	Naphtheno-Olefin	7	7	2	6	1	1	0	26.4	375.1	503		
ethylcyclopentane	Naphthene	7	7	1	7	0	1	0	16.2	376.6	486	58.6	2.0
2,4,4-trimethyl-2-pentene	Olefin	8	8	1	6	1	0	0	18.9	377.1	481		
1,1,3-Trimethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	378.0	471		
2,2-dimethylhexane	Alkane	8	8	0	7	0	0	0	7.0	378.8	462	52.8	2.0
1,3-Cyclopentadiene, 1,2-dimet	Naphtheno-Olefin	7	7	3	5	2	1	0	36.6	379.5	455		
1-Ethylcyclopentene	Naphtheno-Olefin	7	7	2	6	1	1	0	26.4	380.0	451		
Butane, 2,2,3,3-tetramethyl-	Alkane	8	8	0	7	0	0	0	7.0	380.0	451	56.1	2.0
2-Pentene, 3,4,4-trimethyl-	Olefin	8	8	1	6	1	0	0	18.9	381.9	431		
2,5-dimethylhexane	Alkane	8	8	0	7	0	0	0	7.0	382.2	428		
2,4-dimethylhexane	Alkane	8	8	0	7	0	0	0	7.0	382.5	425	56.1	2.0
2,2,3-Trimethylpentane	Alkane	8	8	0	7	0	0	0	7.0	383.0	420		
1-methyl-1-cyclohexene	Naphtheno-Olefin	7	7	2	6	1	1	0	26.4	383.1	419		
C7_Naphtheno-Olefins(1)	Naphtheno-Olefin	7	7	2	6	1	1	0	26.4	383.1	419	61.7	3.0
2-Hexene, 2,4-dimethyl-	Olefin	8	8	1	6	1	0	0	18.9	383.8	413		
toluene	Aromatic	7	7	4	4	0	0	1	39.6	383.7	413		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
3,3-Dimethylhexane	Alkane	8	8	0	7	0	0	0	7.0	384.2	409	175.6	7.7
C8_Mono-Naphthenes(3)	Naphthene	8	8	1	8	0	1	0	18.9	384.5	406		
1-methyl-1,4-cyclohexadiene	Naphtheno-Olefin	7	7	3	5	2	1	0	36.6	384.7	404		
1-butanol	Alkane	4	5	0	4	0	0	0	4.0	390.6	403	22.0	2.5
2-methyl-1-propanol	Alkane	4	5	0	4	0	0	0	4.0	381.1	403	26.2	2.4
2,3-Dimethyl-1-hexene	Olefin	8	8	1	6	1	0	0	18.9	385.2	399	60.9	2.0
1-Heptene, 5-methyl-	Olefin	8	8	1	6	1	0	0	18.9	385.5	397		
2-Hexene, 3,5-dimethyl-	Olefin	8	8	1	6	1	0	0	18.9	386.0	392		
2,3,4-trimethylpentane	Alkane	8	8	0	7	0	0	0	7.0	386.6	387		
C8-Napht-Olefin	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	387.1	383		
2-Hexene, 2,5-dimethyl-	Olefin	8	8	1	6	1	0	0	18.9	387.5	380		
3-Hexene, 2,3-dimethyl-	Olefin	8	8	1	6	1	0	0	18.9	387.5	380		
2,3,3-Trimethylpentane	Alkane	8	8	0	7	0	0	0	7.0	387.9	375		
C8 - Diolefin - 1	Olefin	8	8	2	5	2	0	0	30.8	388.1	374		
2,3-Dimethylhexane	Alkane	8	8	0	7	0	0	0	7.0	388.1	374		
2-Methyl-3-ethylpentane	Alkane	8	8	0	7	0	0	0	7.0	388.1	374	55.2	2.0
4-Methyl-2-heptene	Olefin	8	8	1	6	1	0	0	18.9	388.3	372		
4-Methyl-2-heptene	Olefin	8	8	1	6	1	0	0	18.9	388.4	372		
1c,2c,4-Trimethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	388.4	372		
5,5-Dimethyl-1,3-hexadiene	Olefin	8	8	2	5	2	0	0	30.8	388.9	368		
3-Ethyl-3-Hexene	Olefin	8	8	1	6	1	0	0	18.9	389.1	365		
C8 - IsoOlefin - 4	Olefin	8	8	1	6	1	0	0	18.9	389.3	364		
1t,2c,3-Trimethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	389.4	363		
Cyclopentane, 1,2,4-trimethyl-, (1à,2á,4à)-	Naphthene	8	8	1	8	0	1	0	18.9	389.5	363		
1c,2t,3-Trimethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	389.5	362		
3,4-dimethylhexane	Alkane	8	8	0	7	0	0	0	7.0	389.7	360	48.1	2.0
1c,2t,4-Trimethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	389.8	359		
4-methylheptane	Alkane	8	8	0	7	0	0	0	7.0	390.1	357		
3-Ethylhexane	Alkane	8	8	0	7	0	0	0	7.0	390.6	353		
C8_Iso-Olefins(2)	Olefin	8	8	1	6	1	0	0	18.9	390.6	353		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
1c,2c,3-Trimethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	390.7	352	49.4	2.0
2-Ethylhexene-1	Olefin	8	8	1	6	1	0	0	18.9	390.8	351		
2-methylheptane	Alkane	8	8	0	7	0	0	0	7.0	390.8	351		
C9_Naphtheno-Olefins(3)	Naphtheno-Olefin	9	9	2	8	1	1	0	35.2	391.0	350		
C8_Naphtheno-Olefins(3)	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	391.0	350	67.9	2.1
1,1-dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	391.1	349		
3-Methyl-3-ethylpentane	Alkane	8	8	0	7	0	0	0	7.0	391.1	349		
2,5-Dimethylhexene-2	Olefin	9	9	1	7	1	0	0	21.6	391.6	345		
1,1-Methylethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	392.0	342	48.7	2.0
C8 - IsoOlefin - 5	Olefin	8	8	1	6	1	0	0	18.9	392.0	342		
3-methylheptane	Alkane	8	8	0	7	0	0	0	7.0	392.0	342		
C8 MonoNaph - 1	Naphthene	8	8	1	8	0	1	0	18.9	392.5	338		
C8_Mono-Naphthenes(1)	Naphthene	8	8	1	8	0	1	0	18.9	392.5	338		
1t,4-Dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	392.6	337		
1c,3-Dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	393.0	334		
3c-Ethylmethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	393.0	334		
3t-Ethylmethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	393.0	334		
C8_Iso-Olefins(4)	Olefin	8	8	1	6	1	0	0	18.9	393.1	333		
3-Heptene, 4-methyl-	Olefin	8	8	1	6	1	0	0	18.9	393.1	333		
1,3-dimethyl-c-cyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	393.3	332		
Cyclopentene, 1,2,3-trimethyl-	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	393.5	330		
3-Octene, (Z)-	Olefin	8	8	1	6	1	0	0	18.9	394.0	326		
trans 2-octene	Olefin	8	8	1	6	1	0	0	18.9	394.0	326	56.7	2.0
trans 3-octene	Olefin	8	8	1	6	1	0	0	18.9	394.0	326	58.8	2.0
1,2,4-Trimethylcyclopentane-A	Naphthene	8	8	1	8	0	1	0	18.9	394.2	325	67.6	2.1
1,4-dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	394.2	325		
1,2,4-Trimethylcyclopentane-B	Naphthene	8	8	1	8	0	1	0	18.9	394.3	325		
1-octene	Olefin	8	8	1	6	1	0	0	18.9	394.3	324		
C8_Mono-Naphthenes(4)	Naphthene	8	8	1	8	0	1	0	18.9	394.4	324	56.0	2.0
1,2,3-Trimethylcyclopentene	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	395.1	318		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
2,3-Dimethyl-2-hexene	Olefin	8	8	1	6	1	0	0	18.9	395.1	318	59.8	2.0
t-4-Octene	Olefin	8	8	1	6	1	0	0	18.9	395.3	317		
trans 4-octene	Olefin	8	8	1	6	1	0	0	18.9	395.4	316		
C8 - IsoOlefin - 7	Olefin	8	8	1	6	1	0	0	18.9	395.8	313		
2t-Ethylmethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	395.9	312		
c-Octene-3	Olefin	8	8	1	6	1	0	0	18.9	396.1	311		
C8 MonoNaph - 2	Naphthene	8	8	1	8	0	1	0	18.9	396.4	309		
1,3-dimethyl-t-cyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	396.4	309		
3t-Ethylmethylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	397.1	304		
Cyclopentane, 1-ethyl-2-methyl	Naphthene	8	8	1	8	0	1	0	18.9	397.1	304		
2,2,5-Trimethylhexane	Alkane	9	9	0	8	0	0	0	8.0	397.2	303	42.6	2.0
Cyclopentane, 1-ethyl-2-methyl-	Naphthene	8	8	1	8	0	1	0	18.9	397.3	303		
C8 - Diolefin - 2	Olefin	8	8	2	5	2	0	0	30.8	397.5	301		
t-Octene-2	Olefin	8	8	1	6	1	0	0	18.9	398.0	298		
n-octane	Alkane	8	8	0	7	0	0	0	7.0	398.1	297		
i-Propylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	398.3	295		
c-Octene-2	Olefin	8	8	1	6	1	0	0	18.9	398.5	294		
2,2,4-Trimethylhexane	Alkane	9	9	0	8	0	0	0	8.0	398.6	293		
1,3-dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	399.0	290	67.6	2.1
1c,4-Dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	399.0	290		
1t,2-Dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	399.0	290		
1t,3-Dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	399.0	290		
C8_Mono-Naphthenes(2)	Naphthene	8	8	1	8	0	1	0	18.9	399.0	290		
cis 1,2-dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	399.0	290	65.2	2.0
Cyclohexane, 1,2-dimethyl-	Naphthene	8	8	1	8	0	1	0	18.9	399.0	290		
1,3-Dimethyl-1-cyclohexene	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	399.9	285		
1,4-Dimethyl-1-cyclohexene	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	399.8	285		
C9-Isoparaffin-x	Alkane	9	9	0	8	0	0	0	8.0	399.9	285		
2,3,3-Trimethyl-1-hexene	Olefin	9	9	1	7	1	0	0	21.6	400.3	282		
3,5,5-Trimethylhexene-1	Olefin	9	9	1	7	1	0	0	21.6	400.2	282		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C8 - MonoNaph - 3	Naphthene	8	8	1	8	0	1	0	18.9	400.6	280	60.7	2.0
C9_I-Paraffins(6)	Alkane	9	9	0	8	0	0	0	8.0	401.1	276		
Hexane, 2,4,4-trimethyl-	Alkane	9	9	0	8	0	0	0	8.0	401.1	276		
C8_Mono-Naphthenes(5)	Naphthene	8	8	1	8	0	1	0	18.9	392.5	274		
1-Ethyl-5-methylcyclopentene	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	401.9	272		
C8_Naphtheno-Olefins(5)	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	401.9	272		
3,5-Dimethylhexene	Olefin	8	8	1	6	1	0	0	18.9	402.1	270		
2,3,3-Trimethylhexene-1	Olefin	9	9	1	7	1	0	0	21.6	402.1	270		
t-2,2-Dimethylheptene-3	Olefin	9	9	1	7	1	0	0	21.6	402.2	270		
ethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	402.5	268		
C8 - IsoOlefin - 10	Olefin	8	8	1	6	1	0	0	18.9	402.8	266		
1c,2-Dimethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	402.8	266		
C9_Mono-Naphthenes(1)	Naphthene	9	9	1	9	0	1	0	21.6	402.9	266		
C9_Mono-Naphthenes(2)	Naphthene	9	9	1	9	0	1	0	21.6	402.9	266		
C9_Mono-Naphthenes(31)	Naphthene	9	9	1	9	0	1	0	21.6	427.6	265		
C9_I-Paraffins(5)	Alkane	9	9	0	8	0	0	0	8.0	401.1	262		
C8 - Naph-Olefin - 5	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	403.7	260		
C8_Naphtheno-Olefins(1)	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	404.0	259		
C9 - IsoOlefin - 1	Olefin	9	9	1	7	1	0	0	21.6	404.0	258		
n-Propylcyclopentane	Naphthene	8	8	1	8	0	1	0	18.9	404.1	258		
2,3,5-Trimethylhexane	Alkane	9	9	0	8	0	0	0	8.0	404.5	255		
C9_I-Paraffins(2)	Alkane	9	9	0	8	0	0	0	8.0	404.5	255		
C8_Naphtheno-Olefins(8)	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	404.9	253		
2,2-Dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	405.0	253		
C9_I-Paraffins(3)	Alkane	9	9	0	8	0	0	0	8.0	405.9	248		
1-H-Indene	Aromatic	9	9	6	6	1	1	1	80.0	405.9	247		
C9_I-Paraffins(1)	Alkane	9	9	0	8	0	0	0	8.0	406.1	246		
C9 - MonoNaph - 1	Naphthene	9	9	1	9	0	1	0	21.6	406.3	245		
2,4-Dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	406.7	242		
2,4-Dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	406.8	242		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
2,2,3-Trimethylhexane	Alkane	9	9	0	8	0	0	0	8.0	406.8	242	223.7	9.3
2,2,3,4-Tetramethylpentane	Alkane	9	9	0	8	0	0	0	8.0	407.0	241		
C9_Iso-Olefins(1)	Olefin	9	9	1	7	1	0	0	21.6	407.2	240		
1à,2à,3à,4á-Tetramethylcyclopentane	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
1,1,4-Trimethylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
3-Heptene, 2,6-dimethyl-	Olefin	9	9	1	7	1	0	0	21.6	408.1	235		
C9_Mono-Naphthenes(10)	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
C9_Mono-Naphthenes(12)	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
C9_Mono-Naphthenes(13)	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
C9_Mono-Naphthenes(19)	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
C9_Mono-Naphthenes(5)	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
C9_Mono-Naphthenes(7)	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
C9_Mono-Naphthenes(8)	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
C9_Mono-Naphthenes(9)	Naphthene	9	9	1	9	0	1	0	21.6	408.1	235		
1-Ethyl-2-Methylcyclopentene	Alkane	9	9	0	8	0	0	0	8.0	408.3	234		
Cyclohexene, 1-ethyl-	Naphtheno-Olefin	8	8	2	7	1	1	0	30.8	408.3	234		
2,6-Dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	408.3	233		
3,5-Dimethyl-3-heptene	Olefin	9	9	1	7	1	0	0	21.6	408.9	230		
2,5-Dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	408.9	230		
3,5-Dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	409.1	229		
C9_I-Paraffins(4)	Alkane	9	9	0	8	0	0	0	8.0	409.1	229		
ethylbenzene	Aromatic	8	8	4	5	0	0	1	46.2	409.3	228		
2-Methyloctene-2	Olefin	9	9	1	7	1	0	0	21.6	409.4	228		
3-Heptene, 4-ethyl-	Olefin	9	9	1	7	1	0	0	21.6	409.4	228		
cis-3-Nonene	Olefin	9	9	1	7	1	0	0	21.6	409.5	227		
c-Nonene-3	Olefin	9	9	1	7	1	0	0	21.6	409.5	227		
trans-4-Nonene	Olefin	9	9	1	7	1	0	0	21.6	409.5	227		
C9 Naph-Olefin -1	Naphtheno-Olefin	9	9	2	8	1	1	0	35.2	409.5	227		
3,3-Dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	410.0	225		
Heptane, 3,3-dimethyl-	Alkane	9	9	0	8	0	0	0	8.0	410.3	223		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
2,4-Dimethylheptene-1	Olefin	9	9	1	7	1	0	0	21.6	410.4	222	221.6	9.3
2,6-Dimethylheptene-1	Olefin	9	9	1	7	1	0	0	21.6	410.5	222		
C9 - MonoNaph - 2	Naphthene	9	9	1	9	0	1	0	21.6	410.6	222		
1-Octene, 6-methyl-	Olefin	9	9	1	7	1	0	0	21.6	410.8	221		
C9_Iso-Olefins(5)	Olefin	9	9	1	7	1	0	0	21.6	410.8	221		
Hexane, 2,3,3-trimethyl-	Alkane	9	9	0	8	0	0	0	8.0	411.0	219		
1,3-dimethylbenzene	Aromatic	8	8	4	5	0	0	1	46.2	411.1	219		
C9 - MonoNaph - 3	Naphthene	9	9	1	9	0	1	0	21.6	411.4	217		
Hexane, 3-ethyl-2-methyl-	Alkane	9	9	0	8	0	0	0	8.0	411.5	216		
C9 - MonoNaph - 4	Naphthene	9	9	1	9	0	1	0	21.6	411.6	216		
1,1,3-Trimethylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	411.6	216	211.1	8.8
2,3,4-Trimethylhexane	Alkane	9	9	0	8	0	0	0	8.0	411.6	216		
Cyclohexane, 1,3,5-trimethyl-, (1à,3à,5á)-	Naphthene	9	9	1	9	0	1	0	21.6	412.6	211		
1c,2t,4c-Trimethylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	412.6	211		
1,4-dimethylbenzene	Aromatic	8	8	4	5	0	0	1	46.2	412.8	210		
C9-IsoOlefin-3	Olefin	9	9	1	7	1	0	0	21.6	413.0	209		
2,3-dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	413.6	206	60.2	2.0
3,4-Dimethylheptane	Alkane	9	9	0	8	0	0	0	8.0	413.8	205		
4-Ethylheptane	Alkane	9	9	0	8	0	0	0	8.0	414.4	203		
Pentane, 2,3,3,4-tetramethyl-	Alkane	9	9	0	8	0	0	0	8.0	414.5	202		
4-Methyloctane	Alkane	9	9	0	8	0	0	0	8.0	414.7	201		
C9 - Olefin - 1	Olefin	9	9	1	7	1	0	0	21.6	414.9	200		
C9 - NaphOlefin - 2	Naphtheno-Olefin	9	9	2	8	1	1	0	35.2	415.2	198		
C9_Mono-Naphthenes(29)	Naphthene	9	9	1	9	0	1	0	21.6	415.5	197		
Cyclopentane, 1-methyl-3-(1-methylethyl)-	Naphthene	9	9	1	9	0	1	0	21.6	415.5	197		
1c,3c,5-Trimethylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	415.5	197		
C9_Mono-Naphthenes(6)	Naphthene	9	9	1	9	0	1	0	21.6	415.5	197	415.5	197
Cyclohexane, 1,2,4-trimethyl-,	Naphthene	9	9	1	9	0	1	0	21.6	415.5	197		
C9 - MonoNaph - 5	Naphthene	9	9	1	9	0	1	0	21.6	415.6	197		
2-Methyloctene-1	Olefin	9	9	1	7	1	0	0	21.6	415.7	196		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C9_Iso-Olefins(2)	Olefin	9	9	1	7	1	0	0	21.6	415.8	196	204.8	8.8
C9-isoolefin	Olefin	9	9	1	7	1	0	0	21.6	415.9	195		
trans-1,2-Diethyl cyclopentane	Naphthene	9	9	1	9	0	1	0	21.6	415.9	195		
1,2-dimethylbenzene	Aromatic	8	8	4	5	0	0	1	46.2	416.1	194		
1c,2t,4t-Trimethylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	416.1	194		
Heptane, 3-ethyl-	Alkane	9	9	0	8	0	0	0	8.0	416.1	194		
C9-MonoNaph-6	Naphthene	9	9	1	9	0	1	0	21.6	416.4	193		
2-Methyloctane	Alkane	9	9	0	8	0	0	0	8.0	416.4	193		
3-Methyloctane	Alkane	9	9	0	8	0	0	0	8.0	416.6	192		
t-Nonene-2	Olefin	9	9	1	7	1	0	0	21.6	417.1	189		
C10 - IsoParaffin - 2	Alkane	10	10	0	9	0	0	0	9.0	417.4	189		
C9_Mono-Naphthenes(11)	Naphthene	9	9	1	9	0	1	0	21.6	417.5	188		
trans-1,3-Diethylcyclopentane	Naphthene	9	9	1	9	0	1	0	21.6	417.5	188		
C10 - IsoParaffin - 1	Alkane	10	10	0	9	0	0	0	9.0	417.8	187		
3-Heptene, 4-ethyl-	Olefin	9	9	1	7	1	0	0	21.6	418.0	186		
C9_Iso-Olefins(3)	Olefin	9	9	1	7	1	0	0	21.6		185		
2,3-Dimethylheptene-2	Olefin	9	9	1	7	1	0	0	21.6	418.2	185		
1,1,2-Trimethylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	418.3	184		
C9_Mono-Naphthenes(25)	Naphthene	9	9	1	9	0	1	0	21.6	418.4	184		
C9_Mono-Naphthenes(26)	Naphthene	9	9	1	9	0	1	0	21.6	418.4	184		
C9_Mono-Naphthenes(30)	Naphthene	9	9	1	9	0	1	0	21.6	418.4	184		
1,1,2-Trimethylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	418.4	184		
3-Octyne, 6-methyl-	`	9	9	2	6	2	0	0	35.2	418.5	184		
cis-4-Nonene	Olefin	9	9	1	7	1	0	0	21.6	418.9	182		
t-Nonene-3	Olefin	9	9	1	7	1	0	0	21.6	418.9	182		
4-Nonene	Olefin	9	9	1	7	1	0	0	21.6	418.9	182		
C10_I-Paraffins(24)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(25)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(5)	Alkane	10	10	0	9	0	0	0	9.0	419.8	178		
C10_I-Paraffins(6)	Alkane	10	10	0	9	0	0	0	9.0	419.8	178		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
1-nonene	Olefin	9	9	1	7	1	0	0	21.6	420.1	176	64.4	2.0
2-Methyl-2-octene	Olefin	9	9	1	7	1	0	0	21.6	420.1	176		
C10_I-Paraffins(6)	Alkane	10	10	0	9	0	0	0	9.0		1		
C10_I-Paraffins(7)	Alkane	10	10	0	9	0	0	0	9.0		1		
C10_Iso-Olefins(1)	Olefin	10	10	1	8	1	0	0	24.3		176		
C10_Iso-Olefins(2)	Olefin	10	10	1	8	1	0	0	24.3		176		
Nonane, 4,5-dimethyl-	Alkane	11	11	0	10	0	0	0	10.0		176		
3,3-Diethylpentane	Alkane	9	9	0	8	0	0	0	8.0	420.4	175		
t-2,2,5,5-Tetramethylhexene-3	Olefin	10	10	1	8	1	0	0	24.3	422.0	169		
Cyclohexane, 1-ethyl-3-methyl	Naphthene	9	9	1	9	0	1	0	21.6	422.0	169		
Cyclohexane, 1-ethyl-4-methyl-	Naphthene	9	9	1	9	0	1	0	21.6	422.0	169		
Cyclohexane, 1,2,3-trimethyl-, (1à,2à,3à)-	Naphthene	9	9	1	9	0	1	0	21.6	422.0	169		
Cyclopentane, 1-methyl-2-propyl-	Naphthene	9	9	1	9	0	1	0	21.6	422.0	168		
Heptane, 2,4,6-trimethyl-	Alkane	10	10	0	9	0	0	0	9.0	422.1	168		
2,2,4-trimethylheptane	Alkane	10	10	0	9	0	0	0	9.0	422.3	167		
C10_I-Paraffins(23)	Alkane	10	10	0	9	0	0	0	9.0	422.4	167		
Cyclopentane, 1-methyl-3-(2-methylpropyl)-	Naphthene	10	10	1	10	0	1	0	24.3	422.6	166		
C10_Mono-Naphthenes(11)	Naphthene	10	10	1	10	0	1	0	24.3	422.6	166		
C10_Mono-Naphthenes(12)	Naphthene	10	10	1	10	0	1	0	24.3	422.6	166		
C9 - MonoNaph - 2(1)	Naphthene	9	9	1	9	0	1	0	21.6	422.9	165		
C10_I-Paraffins(2)	Alkane	10	10	0	9	0	0	0	9.0		-		
C9_Mono-Naphthenes(18)	Naphthene	9	9	1	9	0	1	0	21.6	423.4	163		
i-Butylcyclopentane	Naphthene	9	9	1	9	0	1	0	21.6	423.3	163		
1-ethyl-4-t-methylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	423.7	162		
1-Ethyl-4-methylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	424.0	161		
C9_Mono-Naphthenes(21)	Naphthene	9	9	1	9	0	1	0	21.6	424.0	161		
C9_Mono-Naphthenes(23)	Naphthene	9	9	1	9	0	1	0	21.6	424.0	161		
cis-1-Ethyl-3-methyl-cyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	424.0	161		
Cyclohexane, 1-ethyl-4-methyl-, trans-	Naphthene	9	9	1	9	0	1	0	21.6	424.0	161		
C9_Mono-Naphthenes(20)	Naphthene	9	9	1	9	0	1	0	21.6	424.0	161		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C9_Mono-Naphthenes(22)	Naphthene	9	9	1	9	0	1	0	21.6	424.0	161	50.1	2.0
1-Octene, 2,6-dimethyl-	Olefin	10	10	1	8	1	0	0	24.3	424.3	160		
C8 - Naph-Olefin - 1	Alkane	8	8	0	7	0	0	0	7.0	424.3	159		
n-nonane	Alkane	9	9	0	8	0	0	0	8.0	424.8	157		
C9_Mono-Naphthenes(14)	Naphthene	9	9	1	9	0	1	0	21.6	425.0	157	74.7	2.2
C9_Mono-Naphthenes(15)	Naphthene	9	9	1	9	0	1	0	21.6	425.0	157		
C9_Mono-Naphthenes(16)	Naphthene	9	9	1	9	0	1	0	21.6	425.0	157		
isopropylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	425.0	157		
C10-IsoOlefin-4	Olefin	10	10	1	8	1	0	0	24.3	425.2	156	187.6	8.2
1,1-Methylethylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	425.3	156		
C9_Mono-Naphthenes(27)	Naphthene	9	9	1	9	0	1	0	21.6	425.4	156		
C10 Iso-olefin - 5	Olefin	10	10	1	8	1	0	0	24.3	425.5	155		
isopropylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	425.5	155	69.2	2.1
i-Propylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	426.0	153		
C8 - Naph-Olefin - 2	Alkane	8	8	0	7	0	0	0	7.0	426.8	150		
C10 Iso-olefin - 6	Olefin	10	10	1	8	1	0	0	24.3	427.0	149		
2,3-Dimethyloctane	Alkane	10	10	0	9	0	0	0	9.0	427.3	148	69.2	2.1
propylcyclohexane	Naphthene	9	9	1	9	0	1	0	21.6	428.1	145		
3-Heptyne, 5-ethyl-5-methyl-	Olefin	10	10	2	7	2	0	0	39.6	428.5	144		
C10_Mono-Naphthenes(10)	Naphthene	10	10	1	10	0	1	0	24.3	422.6	143		
3,3,5-TrimethylHeptane	Alkane	10	10	0	9	0	0	0	9.0	428.8	143	69.2	2.1
Heptane, 3,3,5-trimethyl-	Alkane	10	10	0	9	0	0	0	9.0	429.0	143		
C9_Mono-Naphthenes(32)	Naphthene	9	9	1	9	0	1	0	21.6	429.1	142		
Cyclohexane, 1-ethyl-2-methyl-, cis-	Naphthene	9	9	1	9	0	1	0	21.6	429.1	142		
2,2-Dimethyloctane	Alkane	10	10	0	9	0	0	0	9.0	429.2	142	69.2	2.1
C10_I-Paraffins(22)	Alkane	10	10	0	9	0	0	0	9.0	434.1	141		
Cyclohexane, 1,1,3,5-tetramethyl-, trans-	Naphthene	10	10	1	10	0	1	0	24.3	429.5	141		
2,6-Dimethyloctane	Alkane	10	10	0	9	0	0	0	9.0	429.5	141		
n-Butylcyclopentane	Naphthene	9	9	1	9	0	1	0	21.6	429.9	139	69.2	2.1
C10-IsoOlefin-7	Olefin	10	10	1	8	1	0	0	24.3	429.9	139		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
2,3,6-trimethylheptane	Alkane	10	10	0	9	0	0	0	9.0	430.0	139		
C10_I-Paraffins(22)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(23)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(4)	Alkane	10	10	0	9	0	0	0	9.0	430.0	139		
C10_I-Paraffins(4)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(8)	Alkane	10	10	0	9	0	0	0	9.0	430.0	139		
Cyclopropane, 1,2-dimethyl-1-pentyl-	Naphthene	10	10	1	10	0	1	0	24.3	430.5	137		
C10 Isoparaffin -1	Alkane	10	10	0	9	0	0	0	9.0	430.8	136		
Diethylcyclohexane	Naphthene	8	8	1	8	0	1	0	18.9	430.9	136		
Heptane, 2,3,5-trimethyl-	Alkane	10	10	0	9	0	0	0	9.0	431.0	135		
3-Hexene, 3-ethyl-2,5-dimethyl-	Olefin	10	10	1	8	1	0	0	24.3	431.4	134		
C9 - MonoNaph - 6	Naphthene	9	9	1	9	0	1	0	21.6	431.5	134		
4-Octene, 2,6-dimethyl-, [S-(Z)]-	Olefin	10	10	1	8	1	0	0	24.3	431.5	134		
C10-n-Olefin	Olefin	10	10	1	8	1	0	0	24.3	431.5	134		
2,7-dimethyloctane	Alkane	10	10	0	9	0	0	0	9.0	431.6	133		
2,5-Dimethyloctane	Alkane	10	10	0	9	0	0	0	9.0	431.6	133		
2,7-Dimethyloctane	Alkane	10	10	0	9	0	0	0	9.0	431.6	133		
3-Nonene, 3-methyl-, (E)-	Olefin	10	10	1	8	1	0	0	24.3	432.2	132		
C10 - IsoOlefin - 8	Olefin	10	10	1	8	1	0	0	24.3	432.3	131		
C9_Naphtheno-Olefins(4)	Naphtheno-Olefin	9	9	2	8	1	1	0	35.2	432.4	131		
3-Methyl-5-ethylheptane	Alkane	10	10	0	9	0	0	0	9.0	432.5	131		
C10_I-Paraffins(20)	Alkane	10	10	0	9	0	0	0	9.0	432.9	130		
C10_I-Paraffins(20)	Alkane	10	10	0	9	0	0	0	9.0		-		
1,2,3,5-t-Tetramethylcyclohex	Naphthene	10	10	1	10	0	1	0	24.3	433.5	127		
C10_I-Paraffins(1)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(10)	Alkane	10	10	0	9	0	0	0	9.0	433.5	127		
C10_I-Paraffins(10)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(11)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(12)	Alkane	10	10	0	9	0	0	0	9.0	433.5	127		
C10_I-Paraffins(12)	Alkane	10	10	0	9	0	0	0	9.0		-		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C10_I-Paraffins(3)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(5)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(7)	Alkane	10	10	0	9	0	0	0	9.0	433.5	127		
C10_I-Paraffins(9)	Alkane	10	10	0	9	0	0	0	9.0	430.0	127		
3-Heptene, 4-propyl-	Olefin	10	10	1	8	1	0	0	24.3	433.6	127		
propylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	433.6	127	235.7	9.9
Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	Naphthene	10	10	1	10	0	1	0	24.3		127		
Cyclopentane, 2-isopropyl-1,3-dimethyl-	Naphthene	10	10	1	10	0	1	0	24.3	433.7	127		
1H-Indene, octahydro-, cis-	Naphthene	9	9	2	10	0	2	0	35.2	434.1	126		
1H-Indene, octahydro-, trans-	Naphthene	9	9	2	10	0	2	0	35.2	434.1	126		
Octane, 3,3-dimethyl-	Alkane	10	10	0	9	0	0	0	9.0	434.1	126		
1-ethyl-3-methylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	434.4	125	278.0	11.1
Heptane, 3-ethyl-2-methyl-	Alkane	10	10	0	9	0	0	0	9.0		123		
1-ethyl-4-methylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	435.1	123	257.1	10.5
C11-Isoparaffin-2	Alkane	11	11	0	10	0	0	0	10.0	436.2	119		
C10_I-Paraffins(13)	Alkane	10	10	0	9	0	0	0	9.0	436.4	119		
C10_I-Paraffins(13)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(14)	Alkane	10	10	0	9	0	0	0	9.0		-		
Octane, 3,4-dimethyl-	Alkane	10	10	0	9	0	0	0	9.0	436.4	119		
Cyclohexane, 1-isopropyl-1-methyl-	Naphthene	10	10	1	10	0	1	0	24.3	436.6	118		
1-ethyl-2-methylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	437.1	117	267.0	11.0
3-Ethyl-3-methylheptane	Alkane	10	10	0	9	0	0	0	9.0	437.3	116		
C10_I-Paraffins(15)	Alkane	10	10	0	9	0	0	0	9.0	437.5	116		
C10_I-Paraffins(15)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10-IsoOlefin-12	Olefin	10	10	1	8	1	0	0	24.3	437.8	115		
5-Methylnonane	Alkane	10	10	0	9	0	0	0	9.0	438.2	113		
Cyclohexane, 1-ethyl-2,3-dimethyl-	Naphthene	10	10	1	10	0	1	0	24.3	438.4	113		
C11-Isoparaffin-1	Alkane	11	11	0	10	0	0	0	10.0	438.6	112		
4-Methylnonane	Alkane	10	10	0	9	0	0	0	9.0	439.1	111		
2-Methylnonane	Alkane	10	10	0	9	0	0	0	9.0	439.1	111		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
4-Methylnonane	Alkane	10	10	0	9	0	0	0	9.0	439.1	111	310.9	12.3
3-Ethyloctane	Alkane	10	10	0	9	0	0	0	9.0	439.6	110		
1,3,5-trimethylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	439.8	109	291.1	11.6
C10 - IsoParaffin - 5	Alkane	10	10	0	9	0	0	0	9.0	440.5	107		
(1,1-dimethylethyl)-benzene	Aromatic	10	10	4	7	0	0	1	59.4	440.9	106	291.1	11.6
3-Methylnonane	Alkane	10	10	0	9	0	0	0	9.0	440.9	106		
C10_I-Paraffins(16)	Alkane	10	10	0	9	0	0	0	9.0	441.0	106	291.1	11.6
C10_I-Paraffins(16)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(17)	Alkane	10	10	0	9	0	0	0	9.0	441.0	106	291.1	11.6
C10_I-Paraffins(17)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(18)	Alkane	10	10	0	9	0	0	0	9.0	441.0	106	291.1	11.6
C10_I-Paraffins(18)	Alkane	10	10	0	9	0	0	0	9.0		-		
C10_I-Paraffins(19)	Alkane	10	10	0	9	0	0	0	9.0	441.0	106	291.1	11.6
C10_I-Paraffins(19)	Alkane	10	10	0	9	0	0	0	9.0		-		
3-Methylnonane	Alkane	10	10	0	9	0	0	0	9.0	441.0	106	291.1	11.6
C10 - IsoParaffin - 6	Alkane	10	10	0	9	0	0	0	9.0	441.0	106		
C10 - MonoNaph - 2	Naphthene	10	10	1	10	0	1	0	24.3	441.1	106	308.3	12.2
1,2,4-trimethylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	441.1	106		
trans-4-Decene	Olefin	10	10	1	8	1	0	0	24.3	441.1	106	308.3	12.2
3-Octene, 4-ethyl-	Olefin	10	10	1	8	1	0	0	24.3	441.4	105		
Cyclohexane, 1-methyl-4-(1-methylethenyl)-, cis-	Naphtheno-Olefin	10	10	2	9	1	1	0	39.6	441.7	104	308.3	12.2
C10 MonoNaphth - 3	Naphthene	10	10	1	10	0	1	0	24.3	441.8	104		
1t-Methyl-2-n-propylcyclohexan	Naphthene	10	10	1	10	0	1	0	24.3	442.2	103	308.3	12.2
1-Isopropyl-3-MECY6	Olefin	10	10	1	8	1	0	0	24.3	442.6	102		
C11 Isoparaffin-1	Alkane	11	11	0	10	0	0	0	10.0	443.6	99	308.3	12.2
C10_Mono-Naphthenes(6)	Naphthene	10	10	1	10	0	1	0	24.3	444.1	98		
C10_Mono-Naphthenes(7)	Naphthene	10	10	1	10	0	1	0	24.3	444.1	98	308.3	12.2
C11 Isoparaffin-2	Alkane	11	11	0	10	0	0	0	10.0	444.3	98		
C10_Mono-Naphthenes(1)	Naphthene	10	10	1	10	0	1	0	24.3	444.5	97	308.3	12.2
C10_Mono-Naphthenes(2)	Naphthene	10	10	1	10	0	1	0	24.3	444.5	97		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
i-Butylcyclohexane	Naphthene	10	10	1	10	0	1	0	24.3	444.4	97	199.1 270.7	8.7 11.0
2,3-Dihydroindene	Aromatic	9	9	6	6	1	1	1	80.0	444.8	96		
C11-Isoparaffin-3	Alkane	11	11	0	10	0	0	0	10.0	444.9	96		
2,4,6-Trimethyloctane	Alkane	11	11	0	10	0	0	0	10.0	445.4	95		
2,2,6-Trimethyloctane	Alkane	11	11	0	10	0	0	0	10.0	445.4	95		
C11_I-Paraffins(2)	Alkane	11	11	0	10	0	0	0	10.0	445.5	95		
C11_I-Paraffins(2)	Alkane	11	11	0	10	0	0	0	10.0		-		
2,5-dimethylnonane	Alkane	11	11	0	10	0	0	0	10.0	445.7	94		
4-Methyldecane	Alkane	11	11	0	10	0	0	0	10.0	446.0	94		
Cyclopentane, (1-methylbutyl)-	Naphthene	10	10	1	10	0	1	0	24.3	446.3	93		
(1-methylpropyl)-benzene	Aromatic	10	10	4	7	0	0	1	59.4	446.4	93		
1,4-diethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	446.4	93		
C11 Isoparaffin - 4	Alkane	11	11	0	10	0	0	0	10.0	446.9	91		
Heptane, 2,2,3,5-tetramethyl-	Alkane	11	11	0	10	0	0	0	10.0	447.0	91		
3-Decene	Olefin	10	10	1	8	1	0	0	24.3	447.0	91		
C10_Mono-Naphthenes(4)	Naphthene	10	10	1	10	0	1	0	24.3	447.1	91	57.2 315.1 257.6	2.0 12.3 10.5
C10_Mono-Naphthenes(5)	Naphthene	10	10	1	10	0	1	0	24.3	447.1	91		
Trans-1,4-diethylcyclohexane	Naphthene	10	10	1	10	0	1	0	24.3	447.1	91		
Octane, 2,3,3-trimethyl-	Alkane	11	11	0	10	0	0	0	10.0	447.4	90		
Octane, 2,6,6-trimethyl-	Alkane	11	11	0	10	0	0	0	10.0	447.4	90		
2,3,3-trimethyloctane	Alkane	11	11	0	10	0	0	0	10.0	447.4	90		
n-decane	Alkane	10	10	0	9	0	0	0	9.0	448.0	89		
C11_I-Paraffins(27)	Alkane	11	11	0	10	0	0	0	10.0	447.4	89		
1,2,3-trimethylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	448.1	89		
1-Methyl-3-i-propylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	448.2	88		
C10_I-Paraffins(8)	Alkane	10	10	0	9	0	0	0	9.0		4		
C10_Mono-Aromatics(1)	Aromatic	10	10	4	7	0	0	1	59.4	448.2	88		
C10_Mono-Aromatics(8)	Aromatic	10	10	4	7	0	0	1	59.4	448.5	88		
(2-methylpropyl)-benzene	Aromatic	10	10	4	7	0	0	1	59.4	448.5	88		
C11 IsoParaffin - 5	Alkane	11	11	0	10	0	0	0	10.0	448.6	88		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
1-isopropyl-4-methylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	449.1	86	330.3	12.9
C11 Isoparaffin-4	Alkane	11	11	0	10	0	0	0	10.0	449.2	86		
C9_Mono-Aromatics(1)	Aromatic	9	9	4	6	0	0	1	52.8	449.3	86		
C11 - MonoNaph - 1	Naphthene	11	11	1	11	0	1	0	27.0	449.4	86		
indan	Aromatic	9	9	5	7	0	1	1	66.4	449.6	85	439.5	16.6
indane	Aromatic	9	9	5	7	0	1	1	66.4	449.6	85	439.5	16.6
2,5,6-Trimethyloctane	Alkane	11	11	0	10	0	0	0	10.0	449.8	85		
Octane, 6-ethyl-2-methyl-	Alkane	11	11	0	10	0	0	0	10.0	450.2	84		
3-Ethylnonane	Alkane	11	11	0	10	0	0	0	10.0	450.6	83		
C11-Isoparaffin-5	Alkane	11	11	0	10	0	0	0	10.0	451.0	83		
Heptane, 2,2,4,6,6-pentamethyl-	Alkane	11	11	0	10	0	0	0	10.0	451.0	83		
C12_Indanes(9)	Aromatic	12	12	5	10	0	1	1	91.3	451.0	82		
C11_Indanes(1)	Aromatic	11	11	5	9	0	1	1	83.0	451.0	82		
C12_Indanes(1)	Aromatic	12	12	5	10	0	1	1	91.3	451.0	82		
C12_Indanes(3)	Aromatic	12	12	5	10	0	1	1	91.3	451.0	82		
C12_Indanes(4)	Aromatic	12	12	5	10	0	1	1	91.3	451.0	82		
C12_Indanes(6)	Aromatic	12	12	5	10	0	1	1	91.3	451.0	82		
C12_Indanes(8)	Aromatic	12	12	5	10	0	1	1	91.3	451.0	82		
C13_Indanes(1)	Aromatic	13	13	5	10	0	1	1	99.6	451.0	82		
1-Methyl-2-i-propylbenzene	Aromatic	10	10	4	4	0	0	1	59.4		82		
Octane, 5-ethyl-2-methyl-	Alkane	11	11	0	10	0	0	0	10.0	451.4	82		
C10_Mono-Naphthenes(3)	Naphthene	10	10	1	10	0	1	0	24.3	451.6	81		
Cyclooctane, 1,2-dimethyl-	Alkane	10	10	1	8	0	1	0	24.3		81		
C8 Naph-Olefin - 6	Alkane	8	8	0	7	0	0	0	7.0	452.1	80		
C10_Mono-Naphthenes(9)	Naphthene	10	10	1	10	0	1	0	24.3	452.5	80		
Octane, 2,3,7-trimethyl-	Alkane	11	11	0	10	0	0	0	10.0	452.5	80		
C11_I-Paraffins(10)	Alkane	11	11	0	10	0	0	0	10.0	452.5	79		
C11_I-Paraffins(10)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(11)	Alkane	11	11	0	10	0	0	0	10.0	452.5	79		
C11_I-Paraffins(11)	Alkane	11	11	0	10	0	0	0	10.0		-		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
Nonane, 2,3-dimethyl-	Alkane	11	11	0	10	0	0	0	10.0		79		
2,2,3-trimethyloctane	Alkane	11	11	0	11	0	0	0	10.0		79		
C11_I-Paraffins(4)	Alkane	11	11	0	10	0	0	0	10.0	452.8	79		
C11_I-Paraffins(4)	Alkane	11	11	0	10	0	0	0	10.0		-		
butylcyclohexane	Naphthene	10	10	1	10	0	1	0	24.3	453.5	77	76.8	2.2
n-butylcyclohexane	Naphthene	10	10	1	10	0	1	0	24.3	453.5	77	76.8	2.2
C11 - IsoParaffin - 6	Alkane	11	11	0	10	0	0	0	10.0	453.8	77		
C11-Isoparaffin-7	Alkane	11	11	0	10	0	0	0	10.0	454.2	76		
indene	Aromatic	9	9	6	6	1	1	1	80.0	454.7	75	467.7	17.8
1,3-diethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	454.8	75	320.9	12.8
2-Undecene, (E)-	Olefin	11	11	1	9	1	0	0	27.0	455.2	74		
5-Undecene	Olefin	11	11	1	9	1	0	0	27.0	455.2	74		
C11_I-Paraffins(26)	Alkane	11	11	0	10	0	0	0	10.0	462.3	74		
5-Methyldecane	Alkane	11	11	0	10	0	0	0	10.0	456.4	72		
n-butylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	456.4	72	245.1	9.9
Nonane, 2,5-dimethyl-	Alkane	11	11	0	10	0	0	0	10.0		72		
Nonane, 3,7-dimethyl-	Alkane	11	11	0	10	0	0	0	10.0	456.4	72		
C11_I-Paraffins(29)	Alkane	11	11	0	10	0	0	0	10.0	456.5	72		
C10_Mono-Aromatics(10)	Aromatic	10	10	4	7	0	0	1	59.4	456.6	71		
1,2-diethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	456.6	71	376.3	14.7
C10_I-Paraffins(9)	Alkane	10	10	0	9	0	0	0	9.0		4		
C10_Mono-Aromatics(2)	Aromatic	10	10	4	7	0	0	1	59.4	456.6	71		
1-Methyl-3-n-propylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	456.8	71		
C11_I-Paraffins(5)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(9)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C13_I-Paraffins(8)	Alkane	13	13	0	12	0	0	0	12.0	457.1	71		
C11_I-Paraffins(1)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(1)	Alkane	11	11	0	10	0	0	0	10.0	457.1	-		
C11_I-Paraffins(12)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(12)	Alkane	11	11	0	10	0	0	0	10.0		-		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C11_I-Paraffins(13)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(13)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(14)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(15)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(15)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(16)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(16)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(17)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(18)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(19)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(19)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(21)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(21)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(22)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(22)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(24)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(24)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(25)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(25)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(3)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(3)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(5)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(6)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(6)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(7)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(7)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(8)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C11_I-Paraffins(8)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(9)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_Mono-Naphthenes(1)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C11_Mono-Naphthenes(2)	Alkane	11	11	0	10	0	0	0	10.0	457.1	71		
C12_I-Paraffins(1)	Alkane	12	12	0	11	0	0	0	11.0	457.1	71		
C12_I-Paraffins(3)	Alkane	12	12	0	11	0	0	0	11.0	457.1	71		
C12_I-Paraffins(4)	Alkane	12	12	0	11	0	0	0	11.0	457.1	71		
C12_I-Paraffins(5)	Alkane	12	12	0	11	0	0	0	11.0	457.1	71		
C12_I-Paraffins(6)	Alkane	12	12	0	11	0	0	0	11.0	457.1	71		
Decane, 2,3,6-trimethyl-	Alkane	13	13	0	12	0	0	0	12.0		71		
Nonane, 3,7-dimethyl-	Alkane	11	11	0	10	0	0	0	10.0		71		
1-Methyl-4-n-propylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	457.4	70		
C11-Isoparaffin-9	Alkane	11	11	0	10	0	0	0	10.0	457.7	70		
1,3-Dimethyl-5-ethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	457.7	69		
C11- Isoparaffin-10	Alkane	11	11	0	10	0	0	0	10.0	458.4	68		
1-Methylindan	Aromatic	10	10	5	8	0	1	1	74.7	458.6	68		
C11 - IsoParaffin - 9	Alkane	11	11	0	10	0	0	0	10.0	458.9	67		
Decane, 5-methyl-	Alkane	11	11	0	10	0	0	0	10.0	459.3	67		
C11-Isoparaffin-8	Alkane	11	11	0	10	0	0	0	10.0	459.4	67		
(1,2-dimethylpropyl)benzene	Aromatic	11	11	4	8	0	0	1	66.0	459.5	67		
C11_Mono-Aromatics(1)	Aromatic	11	11	4	8	0	0	1	66.0	459.4	67		
C11- Isoparaffin - 12	Alkane	11	11	0	10	0	0	0	10.0	459.5	66		
C10_Mono-Aromatics(11)	Aromatic	10	10	4	7	0	0	1	59.4	459.6	66		
1-Methyl-2-n-propylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	459.6	66		
t-Decalin	Naphthene	10	10	2	11	0	2	0	39.6	460.0	66		
1,4,Dimethyl-2-ethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	460.0	66		
C10_Mono-Aromatics(4)	Aromatic	10	10	4	7	0	0	1	59.4	460.0	66		
C10_Mono-Aromatics(5)	Aromatic	10	10	4	7	0	0	1	59.4	460.0	66		
C11_I-Paraffins(20)	Alkane	11	11	0	10	0	0	0	10.0	460.0	66		
C11_I-Paraffins(20)	Alkane	11	11	0	10	0	0	0	10.0		-		
C11_I-Paraffins(23)	Alkane	11	11	0	10	0	0	0	10.0	460.0	66		
C11_I-Paraffins(23)	Alkane	11	11	0	10	0	0	0	10.0		-		
3-Methyldecane	Alkane	11	11	0	10	0	0	0	10.0	460.1	65		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C10_Mono-Aromatics(9)	Aromatic	10	10	4	7	0	0	1	59.4	463.3	65	436.9	16.6
Decane, 4-methyl-	Alkane	11	11	0	10	0	0	0	10.0	460.5	65		
C13_I-Paraffins(7)	Alkane	13	13	0	12	0	0	0	12.0	457.1	64		
(2-methyl-1-propenyl)-benzene	Aromatic	10	10	5	6	1	0	1	74.7	461.0	64		
1,3-Dimethyl-4-ethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	461.0	64		
C12-isoparaffin-1	Alkane	12	12	0	11	0	0	0	11.0	461.6	63		
C11- Isoparaffin-11	Alkane	11	11	0	10	0	0	0	10.0	461.6	63		
C12_I-Paraffins(11)	Alkane	12	12	0	11	0	0	0	11.0	457.1	63		
Benzene, 1-(1,1-dimethylethyl)-3-methyl-	Aromatic	11	11	4	8	0	0	1	66.0	462.0	62		
C11_I-Paraffins(28)	Alkane	11	11	0	10	0	0	0	10.0	462.3	62		
Decane, 3-methyl-	Alkane	11	11	0	10	0	0	0	10.0	462.3	62		
C11- IsoParaffin - 13	Alkane	11	11	0	10	0	0	0	10.0	462.5	61		
1,2-Dimethyl-4-ethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	462.6	61		
1,3-Dimethyl-2-ethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	463.0	61		
tert-Pentylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	463.1	60		
1,3-Dimethyl-2-ethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	463.2	60		
C10_Mono-Aromatics(6)	Aromatic	10	10	4	7	0	0	1	59.4	463.3	60		
1-t-Butyl-2-methylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	463.5	60		
C11_Mono-Aromatics(2)	Aromatic	11	11	4	8	0	0	1	66.0	463.5	60		
C11 - MonoNaph - 2	Naphthene	11	11	1	11	0	1	0	27.0	463.5	60		
4M-1tC4Benz	Aromatic	10	10	4	7	0	0	1	59.4	464.0	59		
t-Decahydronaphthalene	Naphthene	10	10	2	11	0	2	0	39.6	464.0	59		
1,1-Dimethyl Indane	Aromatic	11	11	5	9	0	1	1	83.0	464.1	59		
C11_Iso-Olefins(1)	Olefin	11	11	1	9	1	0	0	27.0	464.8	58		
C12_Iso-Olefins(2)	Olefin	12	12	1	11	1	0	0	29.7		58		
1,2-Dimethyl-3-ethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	465.1	57		
Benzene, 1-ethyl-3-(1-methylethyl)-	Aromatic	11	11	4	8	0	0	1	66.0	465.6	57		
1H-Indene, 1-methyl-	Aromatic	10	10	6	7	1	1	1	90.0	465.8	56		
C10_Indenes(1)	Aromatic	10	10	6	7	1	1	1	90.0	465.8	56		
1-methyl-4-t-butylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	465.9	56	410.8	15.9

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
1-methyl-4-tert-butylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	465.9	56	410.8	15.9
C11_Mono-Aromatics(14)	Aromatic	11	11	4	8	0	0	1	66.0	466.0	56		
1-Methyl-1-n-butylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	466.0	56		
1-Ethyl-2-n-propylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	466.0	56		
c-Decahydronaphthalene	Naphthene	10	10	2	11	0	2	0	39.6	466.0	56		
Indan, 1-methyl-	Aromatic	10	10	5	8	0	1	1	74.7	466.5	55		
Isopentyl benzene	Aromatic	11	11	4	8	0	0	1	66.0	467.0	55		
Benzene, 1,3-dimethyl-5-(1-methylethyl)-	Aromatic	11	11	4	8	0	0	1	66.0	467.0	55		
C11_Mono-Aromatics(3)	Aromatic	11	11	4	8	0	0	1	66.0	467.1	54		
C11_Mono-Aromatics(4)	Aromatic	11	11	4	8	0	0	1	66.0	467.1	54		
2-Methylindan	Aromatic	10	10	5	8	0	1	1	74.7	467.6	54	64.7	2.0
Heptane, 4-ethyl-2,2,6,6-tetramethyl-	Alkane	13	13	0	12	0	0	0	12.0		53		
C12 - Isoparaffin - 2	Alkane	12	12	0	11	0	0	0	11.0	468.5	53		
1-methyl-4-(1-methylpropyl)be	Aromatic	11	11	4	8	0	0	1	66.0	469.0	52		
n-undecane	Alkane	11	11	0	10	0	0	0	10.0	469.0	52		
1,2,4,5-tetramethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	469.1	52	393.0	15.3
Benzene, 1-methyl-4-(2-methylpropyl)-	Aromatic	11	11	4	8	0	0	1	66.0	469.1	52		
Benzene, 1,4-dimethyl-2-(1-methylethyl)-	Aromatic	11	11	4	8	0	0	1	66.0	469.4	51		
Heptane, 5-ethyl-2,2,3-trimethyl-	Alkane	12	12	0	11	0	0	0	11.0	469.9	51		
1-Ethyl-4-i-propylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	470.1	50		
C12_I-Paraffins(10)	Alkane	12	12	0	11	0	0	0	11.0	470.1	50		
C3-Tetralin-2	Aromatic	13	13	5	11	0	1	1	99.6	470.5	50		
C11 - Aromatic - 1	Aromatic	11	11	4	8	0	0	1	66.0	470.7	50		
C11 - Aromatic - 2	Aromatic	11	11	4	8	0	0	1	66.0	471.7	48		
C13_I-Paraffins(9)	Alkane	13	13	0	12	0	0	0	12.0	457.1	48	386.2	14.8
Decane, 2,5-dimethyl-	Alkane	12	12	0	11	0	0	0	11.0	472.0	48		
1,2,3,5-tetramethylbenzene	Aromatic	10	10	4	7	0	0	1	59.4	472.3	48		
Benzene, 2,4-dimethyl-1-(1-methylethyl)-	Aromatic	11	11	4	8	0	0	1	66.0	472.5	47		
Octane, 3-ethyl-2,7-dimethyl-	Alkane	12	12	0	11	0	0	0	11.0	472.6	47		
C11 - MonoNaph - 3	Naphthene	11	11	1	11	0	1	0	27.0	472.9	47		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C12_I-Paraffins(7)	Alkane	12	12	0	11	0	0	0	11.0	473.5	46	353.3	14.0
Decane, 4-ethyl-	Alkane	12	12	0	11	0	0	0	11.0	473.5	46		
1,3-diethyl-5-methyl benzene	Aromatic	9	9	4	6	0	0	1	52.8	473.8	46		
C12 - IsoParaffin - 1	Alkane	12	12	0	11	0	0	0	11.0	474.0	45		
C12 - IsoParaffin - 2	Alkane	12	12	0	11	0	0	0	11.0	474.1	45		
1H-Indene,2,3-dihydro-2,2-dime	Aromatic	11	11	5	9	0	1	1	83.0	474.3	45		
tert-pentyl benzene	Aromatic	11	11	4	8	0	0	1	66.0	474.5	45		
Benzene, 1,3-diethyl-5-methyl-	Aromatic	11	11	4	8	0	0	1	66.0	476.0	43		
C11 - Aromatic - 6	Aromatic	11	11	4	8	0	0	1	66.0		43		
C11_Mono-Aromatics(5)	Aromatic	11	11	4	8	0	0	1	66.0	476.0	43		
C11_Mono-Aromatics(6)	Aromatic	11	11	4	8	0	0	1	66.0	476.0	43		
C11 - Aromatic - 3	Aromatic	11	11	4	8	0	0	1	66.0	476.0	43		
1,3-diisopropylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	476.1	43		
1-Ethyl-2-i-propylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	476.3	43		
1-Ethyl-3-i-propylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	476.4	43		
4-Octene, 2,3,6,7-tetramethyl-	Olefin	12	12	1	10	1	0	0	29.7	476.4	43		
5-Methylindan	Aromatic	10	10	5	8	0	1	1	74.7	476.6	42		
1,2-Di-i-propylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	477.0	42		
1,3-Di-n-propylbenzene	Aromatic	9	9	4	6	0	0	1	52.8	477.0	42		
C12_Mono-Aromatics(7)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
1-Methyl-2-n-butylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
C12_Mono-Aromatics(11)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
C12_Mono-Aromatics(12)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
C12_Mono-Aromatics(13)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
C12_Mono-Aromatics(14)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
C12_Mono-Aromatics(15)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
C12_Mono-Aromatics(17)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
C12_Mono-Aromatics(5)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
C12_Mono-Aromatics(8)	Aromatic	12	12	4	9	0	0	1	72.6	477.1	42		
Decane, 5,6-dimethyl-	Alkane	12	12	0	11	0	0	0	11.0	477.3	42		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
Benzene, (1-methylbutyl)-	Aromatic	11	11	4	8	0	0	1	66.0	477.3	42	255.0	10.5
C12_Mono-Aromatics(18)	Aromatic	12	12	4	9	0	0	1	72.6	478.1	41		
1-Methyl-3-n-butylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	478.2	41		
C11 - Aromatic - 4	Aromatic	11	11	4	8	0	0	1	66.0	478.3	41		
n-pentylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	478.5	40		
1H-Indene, 3-methyl-	Aromatic	10	10	6	7	1	1	1	90.0	471.2	40		
2,4-diethyl-1-methylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	479.0	40		
4-Methylindan	Aromatic	10	10	5	8	0	1	1	74.7	479.2	40		
1,4-diethyl-2-methylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	479.9	39		
C12 - IsoParaffin - 6	Alkane	12	12	0	11	0	0	0	11.0	480.4	38		
s-Pentylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	480.8	38		
Benzene, (1,3-dimethylbutyl)-	Aromatic	12	12	4	9	0	0	1	72.6	480.9	38		
C12 - Isoparaffin - 3	Alkane	12	12	0	11	0	0	0	11.0	481.0	38		
C11 - Aromatic - 10	Aromatic	11	11	5	7	1	0	1	83.0	481.0	38		
1-t-Butyl-3,5-dimethylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	481.0	38		
C12_Mono-Aromatics(2)	Aromatic	12	12	4	9	0	0	1	72.6	481.0	38		
1H-Indene, 2,3-dihydro-1,3-dimethyl-	Aromatic	11	11	5	9	0	1	1	83.0	481.9	37		
C11_Indanes(2)	Aromatic	11	11	5	9	0	1	1	83.0	481.9	37		
Undecane, 2-methyl-	Alkane	12	12	0	11	0	0	0	11.0	482.0	37		
Benzene, 1-methyl-4-(2-methylpropyl)	Aromatic	11	11	4	8	0	0	1	66.0	482.3	36		
C12_I-Paraffins(2)	Alkane	12	12	0	11	0	0	0	11.0	482.4	36		
C11_Mono-Aromatics(8)	Aromatic	11	11	4	8	0	0	1	66.0	483.1	36		
C11 - Aromatic - 7	Aromatic	11	11	4	8	0	0	1	66.0		36		
1,4-Di-i-propylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	483.4	35		
C11-Aromatic-9	Aromatic	11	11	4	8	0	0	1	66.0	484.1	35		
C12 - IsoParaffin - 4	Alkane	12	12	0	11	0	0	0	11.0	484.3	35		
1t-Butyl-4-ethylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	484.6	34		
C12_Mono-Aromatics(3)	Aromatic	12	12	4	9	0	0	1	72.6	484.6	34		
C12-Aromatic-1	Aromatic	12	12	4	9	0	0	1	72.6	486.1	33		
C11_Mono-Aromatics(15)	Aromatic	11	11	4	8	0	0	1	66.0	486.1	33		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
C11_Mono-Aromatics(16)	Aromatic	11	11	4	8	0	0	1	66.0	486.1	33	71.7	2.1
Dimethyl Indene - 1	Aromatic	11	11	6	8	1	1	1	100.0	486.3	33		
1,3,5-Triethylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	487.1	32		
Dimethyl Indene - 2	Aromatic	11	11	6	8	1	1	1	100.0	487.2	32		
Dimethyl Indene - 3	Aromatic	11	11	6	8	1	1	1	100.0	487.6	32		
n-dodecane	Alkane	12	12	0	11	0	0	0	11.0	488.1	31		
2-Ethyl-2,3-dihydro-1H-indene	Aromatic	11	11	5	9	0	1	1	83.0	488.4	31		
Dimethyl Indane - 1	Aromatic	11	11	5	9	0	1	1	83.0	488.4	31		
C11 - IsoParaffin - 10	Alkane	11	11	0	10	0	0	0	10.0	488.4	31		
C10_I-Paraffins(21)	Alkane	10	10	0	9	0	0	0	9.0	489.5	30		
C10_I-Paraffins(21)	Alkane	10	10	0	9	0	0	0	9.0		-		
Dimethyl Indane - 2	Aromatic	11	11	5	9	0	1	1	83.0	489.5	30		
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	Aromatic	12	12	5	10	0	1	1	91.3		30		
C11 - Aromatic - 11	Aromatic	11	11	4	8	0	0	1	66.0	490.5	29		
1,2,4-Triethylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	491.2	29		
Ethyl-1,3,4-trimethyl benzene	Aromatic	11	11	4	8	0	0	1	66.0	491.5	28		
C11 - Aromatic - 12	Aromatic	11	11	4	8	0	0	1	66.0	492.5	28		
1-ethyl-2,4,5-trimethylbenzen	Aromatic	11	11	4	8	0	0	1	66.0	492.7	27		
1-Ethyl-2,4,5-Trimethylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	492.7	27		
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	Aromatic	12	12	4	9	0	0	1	72.6	493.4	27		
Benzene, 1-(1-methylethenyl)-4-(1-methylethyl)-	Aromatic	12	12	5	8	1	0	1	91.3	493.5	27		
C12_Mono-Aromatics(10)	Aromatic	12	12	5	8	1	0	1	91.3	493.5	27		
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	Aromatic	11	11	5	9	0	1	1	83.0	493.6	27		
Naphthalene, 1,2,3,4-tetrahydr	Aromatic	11	11	5	9	0	1	1	83.0	493.7	27		
C11_Mono-Aromatics(10)	Aromatic	11	11	5	7	1	0	1	83.0	494.3	26		
naphthalene	Aromatic	10	10	7	6	0	0	2	105.3	494.6	26	466.1	8.4
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	Aromatic	12	12	5	10	0	1	1	91.3	494.6	26		
C11-Aromatic-14	Aromatic	11	11	4	8	0	0	1	66.0	494.7	26		
C11 - Aromatic - 13	Aromatic	11	11	4	8	0	0	1	66.0	494.8	26		
1H-Indene, 1-ethyl-2,3-dihydro-	Aromatic	11	11	5	9	0	1	1	83.0	495.1	26		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
1,6-Dimethyl Indan	Aromatic	11	11	5	9	0	1	1	83.0	495.2	26	246.7	9.9
C11 - Aromatic - 14	Aromatic	11	11	4	8	0	0	1	66.0	495.5	25		
C13_I-Paraffins(4)	Alkane	13	13	0	12	0	0	0	12.0	495.5	25		
C13_I-Paraffins(5)	Alkane	13	13	0	12	0	0	0	12.0	495.5	25		
Decane, 2,3,4-trimethyl-	Alkane	13	13	0	12	0	0	0	12.0	495.5	25		
Decane, 2,3,5-trimethyl-	Alkane	13	13	0	12	0	0	0	12.0	495.5	25		
Decane, 2,3,8-trimethyl-	Alkane	13	13	0	12	0	0	0	12.0	495.5	25		
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	Aromatic	12	12	4	9	0	0	1	72.6	495.6	25		
Undecane, 2,7-dimethyl-	Alkane	13	13	0	12	0	0	0	12.0	496.0	25		
Undecane, 2,8-dimethyl-	Alkane	13	13	0	12	0	0	0	12.0	496.0	25		
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	Aromatic	12	12	5	10	0	1	1	91.3	496.1	25		
5-Ethyl Indane	Aromatic	11	11	5	9	0	1	1	83.0	497.7	24		
C2 Indane - 1	Aromatic	11	11	5	9	0	1	1	83.0	497.8	24		
Dodecane, 6-methyl-	Alkane	13	13	0	12	0	0	0	12.0	498.0	24		
1H-Indene, 2,3-dihydro-4,6-dimethyl-	Aromatic	11	11	5	9	0	1	1	83.0	498.3	23		
C11-Aromatic-15	Aromatic	11	11	4	8	0	0	1	66.0	498.3	23		
C12 - Aromatic - 1	Aromatic	12	12	4	9	0	0	1	72.6	498.3	23		
C12 - Aromatic - 10	Aromatic	12	12	5	8	1	0	1	91.3	498.5	23		
C12 - Aromatic - 4	Aromatic	12	12	4	9	0	0	1	72.6	498.9	23		
C12 - Aromatic - 2	Aromatic	12	12	4	9	0	0	1	72.6	499.0	23		
n-hexylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	499.1	23		
Trimethyl Indene - 3	Aromatic	12	12	6	9	1	1	1	110.0	499.3	23		
C12 - Aromatic - 3	Aromatic	12	12	4	9	0	0	1	72.6	499.7	23		
4,7-Dimethyl Indane	Aromatic	11	11	5	9	0	1	1	83.0	499.7	23		
1-Methyl-4-n-pentylbenzene	Aromatic	12	12	4	9	0	0	1	72.6	499.8	22		
C12 - Aromatic - 5	Aromatic	12	12	4	9	0	0	1	72.6	499.9	22		
methyl-tetralin	Aromatic	11	11	5	9	0	1	1	83.0	500.5	22		
1H-Indene, 2,3-dihydro-5,6-dimethyl-	Aromatic	11	11	5	9	0	1	1	83.0	500.8	22		
C3-Indane-2	Aromatic	12	12	5	10	0	1	1	91.3	501.1	22		
4,7-DimethylIndane	Aromatic	11	11	5	9	0	1	1	83.0	501.1	22		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
4,7-Dimethyl Indan	Aromatic	11	11	5	9	0	1	1	83.0	501.1	22	481.8	18.4
Trimethyl Indene - 4	Aromatic	12	12	6	9	1	1	1	110.0	501.2	22		
C13 - Aromatic - 2	Aromatic	13	13	8	6	4	0	1	160.8	501.3	22		
Trimethyl Indene - 2	Aromatic	12	12	6	9	1	1	1	110.0	501.5	21		
Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-	Aromatic	12	12	5	8	1	0	1	91.3	501.7	21		
1-H-Indene,1-3-dimethyl	Aromatic	11	11	6	8	1	1	1	100.0	502.0	21		
pentamethylbenzene	Aromatic	11	11	4	8	0	0	1	66.0	502.1	21		
C13_I-Paraffins(6)	Alkane	13	13	0	12	0	0	0	12.0	502.5	21		
Undecane, 3-ethyl-	Alkane	13	13	0	12	0	0	0	12.0	496.0	21		
C12 - Aromatic - 7	Aromatic	12	12	4	9	0	0	1	72.6	502.6	21		
C12 - Aromatic -8	Aromatic	12	12	4	9	0	0	1	72.6	503.3	20	805.8	30.5
Diimethyl Indene - 2	Aromatic	11	11	6	8	1	1	1	100.0	503.3	20		
acenaphthene	Aromatic	12	12	8	9	0	1	2	147.4	504.3	20		
Trimethyl Indene - 5	Aromatic	12	12	6	9	1	1	1	110.0	504.6	20		
Dimethyl Indane - 3	Aromatic	11	11	5	9	0	1	1	83.0	504.9	19		
C13 - IsoParaffin - 1	Alkane	13	13	0	12	0	0	0	12.0	505.2	19		
Benzene, 1-ethyl-4-(2-methylpropyl)-	Aromatic	12	12	4	9	0	0	1	72.6	484.1	19		
1,3,5-trimethyl-2-propylbenze	Aromatic	12	12	4	9	0	0	1	72.6	505.3	19		
Trimethyl Indene - 6	Aromatic	12	12	6	9	1	1	1	110.0	505.4	19		
Dimethyl Indane - 4	Aromatic	11	11	5	9	0	1	1	83.0	505.7	19		
Benzene, (2,4-dimethylpentyl)-	Aromatic	13	13	4	10	0	0	1	79.2	506.0	19	18	
1-H-Indene-1-Ethyl	Aromatic	11	11	6	2	1	1	1	100.0		19		
1-methyl-2-N-hexylbenzene	Aromatic	13	13	4	10	0	0	1	79.2	507.1	18		
Trimethyl Indene - 7	Aromatic	12	12	6	9	1	1	1	110.0	507.5			
n-Tridecane	Alkane	13	13	0	12	0	0	0	12.0	507.6	18		
1,1,3-Trimethyl Indan	Aromatic	12	12	5	10	1	0	1	91.3	507.9	18		
C13_I-Paraffins(1)	Alkane	13	13	0	12	0	0	0	12.0	508.5	18		
C13_I-Paraffins(2)	Alkane	13	13	0	12	0	0	0	12.0	508.5	18		
C13_I-Paraffins(3)	Alkane	13	13	0	12	0	0	0	12.0	508.5	18		
C13 - IsoParaffin - 2	Alkane	13	13	0	12	0	0	0	12.0	508.9	17		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
1H-Indene, 2,3-dihydro-1,4,7-trimethyl-	Aromatic	12	12	5	10	0	1	1	91.3	509.5	17	649.1	24.7
Trimethyl Indane - 4	Aromatic	12	12	5	10	0	1	1	91.3	509.7	17		
Trimethyl Indene - 8	Aromatic	12	12	6	9	1	1	1	110.0	510.5	17		
C12 - Aromatic - 11(1)	Aromatic	12	12	4	9	0	0	1	72.6	511.8	16		
C12 - Aromatic - 11	Aromatic	12	12	4	9	0	0	1	72.6	511.8	16		
Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-	Aromatic	12	12	5	10	0	1	1	91.3	512.8	15		
1-methylnaphthalene	Aromatic	11	11	7	7	0	0	2	117.0	513.0	15		
2-methylnaphthalene	Aromatic	11	11	7	7	0	0	2	117.0	513.1	15		
C3-tetralin	Aromatic	13	13	5	11	0	1	1	99.6	513.3	15		
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	Aromatic	12	12	5	10	0	1	1	91.3	513.5	15		
6-ethylTetralin	Aromatic	12	12	5	10	0	1	1	91.3	514.4	15	649.1	24.7
1H-Indene, 2,3-dihydro-1,1,4-trimethyl-	Aromatic	12	12	5	10	0	1	1	91.3	517.6	13		
1-Methyl-4-Hexylbenzene	Aromatic	13	13	4	10	0	0	1	79.2	518.8	13		
1,4-dimethyl-1,2,3,4-tetrahyd	Aromatic	12	12	5	10	0	1	1	91.3	520.3	12		
C13-Aromatic-2	Aromatic	13	13	4	10	0	0	1	79.2	520.5	12		
6-ethyl-1,2,3,4-tetrahydronap	Aromatic	12	12	5	10	0	1	1	91.3	520.7	12		
C14-Isoparaffin-1	Alkane	14	14	0	13	0	0	0	13.0	521.6	12		
1H-Indene, 2,3-dihydro-4-propyl-	Aromatic	12	12	5	10	0	1	1	91.3	522.0	12		
Indane,4,5,7-trimethyl	Aromatic	12	12	5	10	0	1	1	91.3		12		
C13 - IsoParaffin - 6	Alkane	13	13	0	12	0	0	0	12.0	523.0	11		
C12-Aromatic-8	Aromatic	12	12	4	9	0	0	1	72.6	524.1	11	649.1	24.7
n-Tetradecane	Alkane	14	14	0	13	0	0	0	13.0	525.1	11		
C2-Tetralin-2	Aromatic	12	12	5	10	0	1	1	91.3	525.6	11		
5-Ethyltetralin	Aromatic	12	12	5	10	0	1	1	91.3	526.3	10		
C13_Mono-NaphtheneS(1)	Naphthene	13	13	1	13	0	1	0	32.4	527.0	10		
C13-Mono-Naphthene-1	Naphthene	13	13	1	13	0	1	0	32.4	527.0	10		
C13 - IsoParaffin - 7	Alkane	13	13	0	12	0	0	0	12.0	527.0	10		
C13-Aromatic-3	Aromatic	13	13	4	10	0	0	1	79.2	527.5	10		
Naphthalene, 1,2,3,4-tetrahydro-5,6-dimethyl-	Aromatic	12	12	5	10	0	1	1	91.3	527.8	10		
C13-Aromatic-4	Aromatic	13	13	4	10	0	0	1	79.2	528.0	10		

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
biphenyl	Aromatic	12	12	8	7	0	0	2	128.7	528.1	10	612.5	22.9
1-Methyl-3-Hexylbenzene	Aromatic	13	13	4	10	0	0	1	79.2	528.5	10		
propyl tetralin	Aromatic	13	13	5	11	0	1	1	99.6	528.8	10		
5-ethyl-1,3-dimethyl Indane	Aromatic	13	13	5	11	0	1	1	99.6	530.8	9		
2-ethylnaphthalene	Aromatic	12	12	7	8	0	0	2	128.7	530.9	9	701.3	26.6
2,2'-dimethylbiphenyl	Aromatic	14	14	8	9	0	0	2	152.1	531.0	9	983.5	36.9
C14_Mono-Aromatics(2)	Aromatic	14	14	8	7	4	0	1	174.2	531.0	9		
C3 Indane - 6	Aromatic	12	12	5	10	0	1	1	91.3	531.1	9		
Dimethylnaphthalene-3	Aromatic	12	12	7	8	0	0	2	128.7	532.0	9		
1-ethylnaphthalene	Aromatic	12	12	7	8	0	0	2	128.7	532.2	9	732.7	27.4
Dimethylnaphthalene-4	Aromatic	12	12	7	8	0	0	2	128.7	533.3	8		
2,6-dimethylnaphthalene	Aromatic	12	12	7	8	0	0	2	128.7	535.1	8	774.5	29.2
Naphthalene,1,7-dimethyl	Aromatic	12	12	7	8	0	0	2	128.7	535.7	8		
Naphthalene, 1,7-dimethyl-	Aromatic	12	12	7	8	0	0	2	128.7	536.0	8		
1,3-dimethylnaphthalene	Aromatic	12	12	7	8	0	0	2	128.7	536.1	8	743.1	28.0
Naphthalene,2,7 dimethyl	Aromatic	12	12	7	8	0	0	2	128.7	536.2	8		
Dimethylnaphthalene-5(1)	Aromatic	12	12	7	8	0	0	2	128.7	536.2	8		
Dimethylnaphthalene-5	Aromatic	12	12	7	8	0	0	2	128.7	536.2	8		
Naphthalene, 2,3,6-trimethyl-	Aromatic	13	13	7	9	0	0	2	140.4	536.7	8		
Dimethylnaphthalene - 6	Aromatic	12	12	7	8	0	0	2	128.7	537.0	7		
Naphthalene, 1,6-dimethyl-	Aromatic	12	12	7	8	0	0	2	128.7	537.2	7		
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	Aromatic	13	13	5	11	0	1	1	99.6	538.0	7		
1,5-dimethylnaphthalene	Aromatic	12	12	7	8	0	0	2	128.7	538.7	7	779.7	29.3
C13_Naphthalenes(2)	Aromatic	13	13	7	9	0	0	2	140.4	540.0	7		
C13_Naphthalenes(5)	Aromatic	13	13	7	9	0	0	2	140.4	540.0	7		
Naphthalene, 2-(1-methylethyl)-	Aromatic	13	13	7	9	0	0	2	140.4	540.0	7		
4-methylbiphenyl	Aromatic	13	13	8	8	0	0	2	140.4	540.9	7	769.3	28.7
1,2-dimethylnaphthalene	Aromatic	12	12	7	8	0	0	2	128.7	541.1	7	743.1	28.0
1,4-dimethylnaphthalene	Aromatic	12	12	7	8	0	0	2	128.7	541.6	6	711.8	26.7
2,3-dimethylnaphthalene	Aromatic	12	12	7	8	0	0	2	128.7	542.0	6	748.4	28.0

Compound Name	Functional Group	yTerm Calculation								Standardized		Pfefferle Lab	
		CN	CON	DBE	SBs	nonDBs	nonArom-Rings	Arom-Rings	yTerm	BP (K)	VP443K (kPa)	YSI	YSI Error
Dimethylnaphthalene-6	Aromatic	12	12	7	8	0	0	2	128.7	543.0	6	779.7	29.3
Naphthalene, 2-ethenyl-	Aromatic	12	12	8	7	1	0	2	147.4		6		
Naphthalene, 1,8-dimethyl-	Aromatic	12	12	7	8	0	0	2	128.7	543.8	6		
n-Pentadecane	Alkane	15	15	0	14	0	0	0	14.0	543.8	6		
3-methylbiphenyl	Aromatic	13	13	8	8	0	0	2	140.4	545.8	6		
1,1'-Biphenyl, 2,3'-dimethyl-	Aromatic	14	14	8	9	0	0	2	152.1	546.0	6		
Naphthalene, 1-propyl-	Aromatic	13	13	7	9	0	0	2	140.4	548.5	5		
1,1'-Biphenyl, 2,4'-dimethyl-	Aromatic	14	14	8	9	0	0	2	152.1	554.0	4		
C14_Mono-Aromatics(1)	Aromatic	14	14	8	7	4	0	1	174.2	554.0	4		
C13_Naphthalenes(3)	Aromatic	13	13	7	9	0	0	2	140.4	554.3	4		
Naphthalene, 1,4,6-trimethyl-	Aromatic	13	13	7	9	0	0	2	140.4	554.3	4		
Benzene, 1-methyl-4-(phenylmethyl)-	Aromatic	14	14	7	10	0	0	2	152.1	559.2	4		
C14_Naphthalenes(1)	Naphthene	14	14	7	10	0	0	2	152.1	552.2	4		
1,1'-Biphenyl, 3,4'-dimethyl-	Aromatic	14	14	8	9	0	0	2	152.1	557.3	4		
C14_Mono-Aromatics(3)	Aromatic	14	14	8	7	4	0	1	174.2	557.3	4		
Azulene, 4,6,8-trimethyl-	Aromatic	13	13	6	3	0	0	2	140.4		4	931.3	52.9
n-Hexadecane	Alkane	16	16	0	15	0	0	0	15.0	559.7	4		
C13_Naphthalenes(4)	Aromatic	13	13	7	9	0	0	2	140.4	560.0	4		
Naphthalene, 1,6,7-trimethyl-	Aromatic	13	13	7	9	0	0	2	140.4	560.0	4		
C13_Naphthalenes(6)	Aromatic	13	13	7	9	0	0	2	140.4	560.0	4		
C13_Naphthalenes(7)	Aromatic	13	13	7	9	0	0	2	140.4	560.0	4		
3,3'-dimethylbiphenyl	Aromatic	14	14	8	9	0	0	2	152.1	562.5	3		
Naphthalene, 1,4,5-trimethyl-	Aromatic	13	13	7	9	0	0	2	140.4	563.5	3		
4-ethylbiphenyl	Aromatic	14	14	8	9	0	0	2	152.1	564.2	3		
C1-Indane - 1	Alkane	10	10	0	9	0	0	0	9.0		3		
Naphthalene, 2,6-diethyl	Aromatic	14	14	7	10	0	0	2	152.1	567.8	3	811.1	30.5

APPENDIX B

METHODOLOGY FOR ESTIMATING PME

B.1 Estimation Methodology

Given the mathematical form for PME shown in this main body of the report and reproduced in Eq. B-1 below, it is clear that the usual approach by which least squares regression is used to estimate empirical coefficients cannot be applied to PME. The main problem is that the exponent α (for VP in the denominator) is present in each term of the summation over the compounds i contained in a fuel. There is no feasible mathematical manipulation of the equation that will extract the empirical coefficients into a linearized equation suitable for direct estimation.

$$\text{PME} = \left(\frac{43.4}{\text{LHV}} \right) \cdot [N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}]^\beta \quad (\text{B-1})$$

where: $\alpha = \{ \alpha_{E0}, \alpha_{E10}, \alpha_{E20} \}$

$$f(EtOH) = \alpha_{E0} + \Delta\alpha \cdot EtOH_{VOL\%}$$

LHV = Lower Heating Value

The development process for the PME formulation is shown in Table B-1. It begins with PME-B for SIDI vehicles and moved in stages through PME-A for SIDI vehicles and PME-A for PFI vehicles. For PME-B, the empirical coefficients are the exponents $\alpha = \{ \alpha_{E0} \text{ and } \alpha_{E10} \}$ for the E0 and E10 fuels in the E-94-2 dataset. To assure linearity of PME-B with LA92 Phase I PM emissions of the SIDI vehicles, the α values were estimated under the constraint that $\beta = 1.00$. Then, to put both the Honda PMI and PME-B on the same scale, N_{TECH} was determined by calculation so that a fuel with Honda PMI of 1.00 would be expected to have a PME-B value of 1.00. The iterative estimation process for $\alpha = \{ \alpha_{E0} \text{ and } \alpha_{E10} \}$ is described below.

Table B-1
Development Process for the PME Formulation

PME-B for SIDI Vehicles (SSI DHA)	$PM_{Ph I} = A_{VEH} \cdot \left(\frac{43.4}{\text{LHV}} \right) \cdot [\underbrace{N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}}_{\beta=1}]^{\beta=1}$
PME-A for SIDI Vehicles (ASTM DHA)	$PM_{Ph I} = A_{VEH} \cdot \left(\frac{43.4}{\text{LHV}} \right) \cdot [N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}]^{\beta=1.17}$
PME-A for PFI Vehicles (ASTM DHA)	$PM_{Ph I} = A_{VEH} \cdot \left(\frac{43.4}{\text{LHV}} \right) \cdot [N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(EtOH)}}]^{\beta=1.17}$
Note: Green font denotes empirically estimated parameters; the red bracket and arrow indicate parameters adopted from prior formulations.	

Once PME-B was determined, PME-A for SIDI vehicles was determined by adopting the term and coefficients inside the square brackets from PME-B and estimating the exponent β to map PME-A into equivalents for PME-B. The term within the square brackets can be referred to as PMI_Y to indicate that it is an extension of the Honda PMI based on the YSI Version 2 database before its adjustment for energy content. The process for estimating β is a direct parallel to the iterative process for α .

Given the result $\beta=1.17$ for PME-A for SIDI vehicles, this β value was adopted for the PME-A formulation for PFI vehicles, since only ASTM DHAs were available for the fuels in the EPAAct dataset. Then, the estimation processed for the α exponents in PME-B was used to estimate an expanded slate of exponents $\alpha=\{\alpha_{E0}, \alpha_{E10}, \alpha_{E20}\}$ for the EPAAct fuels under the assumption that α_{E15} lay half-way between α_{E10} and α_{E20} . The process for estimating $\alpha=\{\alpha_{E0}, \alpha_{E10}, \alpha_{E20}\}$ was the same as for PME-B but expanded to cover three different α values.

The α coefficients of the PME formulation should be thought of as constants for which values are determined iteratively in which one seeks α values such that with $\beta=1.00$ the PME-B values are linearly proportional to LA92 Phase I PM emissions.

The iterative process is straightforward. For illustration, it is described below assuming that only one α coefficient needs to be estimated, as would be true in a dataset of only E0 or E10 fuels.

1. A starting value $\alpha=1.0$ is chosen from the Honda Eq. Then, PME-B is calculated for the E-94-2 experimental fuels assuming $\beta=1.00$. Conventional regression analysis is used to estimate the L coefficient in Eq. B-2:

$$\ln(\text{LA92 Phase I PM}_{i,k}) = A_k + L \cdot \text{PME}_i \quad (\text{B-2})$$

where i = fuel and k = vehicle. The log form is used by convention in emissions analysis to recognize that emissions variability increases with average emissions level. The $\{\alpha, L\}$ pair is retained.

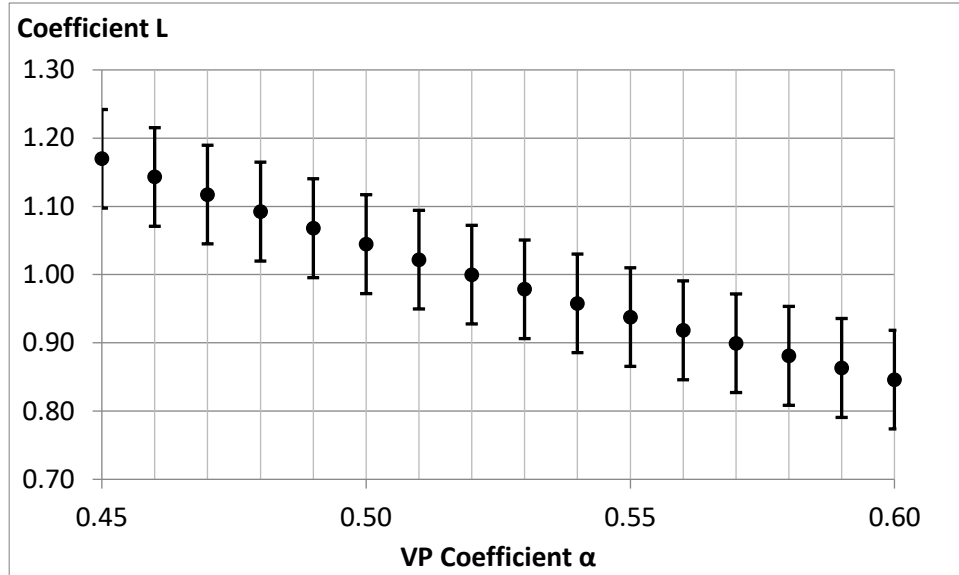
2. A new value for α is chosen by some means, including an arbitrary step in one direction, and Step 1 is repeated. The new $\{\alpha, L\}$ pair is retained.

As different α values are explored, one sees that the linearity parameter L in Eq. B-2 varies across values above and below $L=1.00$. The objective is to find the α value that produces $L=1.00$. In practice, it was generally possible to achieve $L = 1.000 \pm 0.005$, meaning linearity to better than two decimal places.

Figure B-1 illustrates this iterative process for determining α using the portion of a “sweep” between $\alpha=0.45$ and $\alpha=0.60$. The value $\alpha=0.52$ gives the best linearity. The error bars are the standard errors for L estimated in the regression analysis; these are approximately ± 0.08 in the figure. The error bars are the best indicator of the uncertainty in linearization and can be interpreted for this illustration as meaning that LA92 Phase I PM emissions should

be linear with PME-B to within $\pm 8\%$. The α values themselves should be thought of as constants as there is no accepted method for determining a standard error or other measure of uncertainty.

Figure B-1
Iterative Process for Determining the α Coefficient



A similar process was followed when estimating either two or three different α values for the datasets that contained E0 and E10 fuels (E-94-2) or E0, E10, and E15-E20 fuels (EPAAct). For E-94-2, Eq. B-2 was expanded to have two linearity coefficients $\{L_{E0}, L_{E10}\}$ for the E0 and E10 fuels. A search process was followed to find a center point α_0 that gave $L \sim 1.00$. Then, a 3×3 grid was searched around a center point $\{\alpha_{E0}, \alpha_{E10}\} = \{\alpha_0, \alpha_0\} \pm \{\Delta\alpha_{E0}, \Delta\alpha_{E10}\}$. From the 3×3 grid values, values for $\{\alpha_{E0}, \alpha_{E10}\}$ were determined that produced $L_{E0}=1.00$ and $L_{E10}=1.00$ simultaneously.

For EPAAct, Eq. B-2 was expanded to have three linearity coefficients $\{L_{E0}, L_{E10}, L_{E20}\}$ for the E0, E10, and E20 fuels and a $3 \times 3 \times 3$ grid was searched around $\{\alpha_{E0}, \alpha_{E10}, \alpha_{E20}\} = \{\alpha_0, \alpha_0, \alpha_0\} \pm \{\Delta\alpha_{E0}, \Delta\alpha_{E10}, \Delta\alpha_{E20}\}$. The smaller number of E15 fuels were treated by assuming their α value fell halfway between α_{E10} and α_{E20} . From the $3 \times 3 \times 3$ grid values, values for $\{\alpha_{E0}, \alpha_{E10}, \alpha_{E20}\}$ were determined that produced $L_{E0}=1.00$, $L_{E10}=1.00$ and $L_{E20}=1.00$, simultaneously.

B.2 Performance Methodology

The performance of the PME-B and PME-A indices were evaluated by using them to predict LA92 Phase I PM emissions under the assumption that they are linearly related to PM emissions. This was done by fitting Eq. B-3:

$$\ln(\text{Phase I PM}_{i,k}) = A_k + 1 \cdot \text{PME}_i \quad (\text{B-3})$$

where i = fuel and k = vehicle. Note that Eq. B-3 replaces the linearity coefficient L with a fixed value of 1.00 to test the PME formulation under the assumption of linearity. The NLIN non-linear regression package in SAS was used for the estimation because it permitted direct estimation of Eq. B-3 without the re-arrangement needed to use the GLM package for linear regression.

APPENDIX C

PME VALUES FOR THE EXPERIMENTAL FUELS

Table C-1
PME Values for Experimental Fuels in CRC
Emission Studies

Program	Fuel	PME-A	PME-B
E94-2	A	1.27	1.25
	B	1.95	1.93
	E	1.13	1.08
	F	1.75	1.72
	C	1.29	1.21
	D	1.92	1.82
	G	1.11	1.08
	H	1.69	1.69
E94-3	A-3	1.05	1.12
	B-3	1.67	1.74
	E-3	1.04	1.10
	F-3	1.59	1.65
E-129	FUELC	0.00	1.06
	ETOH10	1.06	1.07
	ETOH15	1.03	1.05
	IBUT16	0.86	0.89
	IBUT24	0.88	0.81
	MTBE19	0.84	0.84
	MTBE29	0.75	0.75

Table C-2
PME Values for Experimental Fuels in the EPAct
Emission Study

Program	Fuel	PME-A	PME-B
EPAct	Fuel 1	0.89	PME-B Values Not Determined because SSI DHAs are not available for the fuels.
	Fuel 2	1.15	
	Fuel 3	0.89	
	Fuel 4	1.25	
	Fuel 5	1.39	
	Fuel 6	1.23	
	Fuel 7	0.90	
	Fuel 8	0.89	
	Fuel 9	1.86	
	Fuel 10	2.09	
	Fuel 11	1.47	
	Fuel 12	2.14	
	Fuel 13	1.84	
	Fuel 14	1.16	
	Fuel 15	1.26	
	Fuel 16	1.39	
	Fuel 20	0.99	
	Fuel 21	1.72	
	Fuel 22	0.98	
	Fuel 23	1.48	
	Fuel 24	1.35	
	Fuel 25	2.32	
	Fuel 26	2.23	
	Fuel 27	1.24	
	Fuel 28	1.50	
	Fuel 30	1.66	
	Fuel 31	2.07	

