CRC Report No. AVFL-24

FACE GASOLINES AND BLENDS WITH ETHANOL: DETAILED CHARACTERIZATION OF PHYSICAL AND CHEMICAL PROPERTIES

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FACE Gasolines and Blends with Ethanol: Detailed Characterization of Physical and Chemical Properties

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ACRONYMS

API	American Petroleum Institute
ASTM International	Formerly the American Society for Testing and Materials
AVFL	Advanced Vehicle, Fuel, and Lubricants (CRC)
COA	certificate of analysis
CPChem	Chevron Phillips Chemical Co.
CRC	Coordinating Research Council
DHA	detailed hydrocarbon analysis
FACE	Fuels for Advanced Combustion Engines (CRC)
FBP	final boiling point
FIA	fluorescent indicator adsorption
FID	flame ionization detector
GC	gas chromatography/chromatographic
IBP	initial boiling point
MON	Motor Octane Number
n-	normal (as in normal paraffins)
PAH	polycyclic aromatic hydrocarbon
PIONA	paraffins, isoparaffins, olefins, naphthenes, and aromatics
RON	Research Octane Number
RVP	Reid Vapor Pressure
S	gasoline sensitivity (=RON-MON)
SFC	supercritical fluid chromatography
vol.%	volume %
wt.%	weight %

ACKNOWLEDGMENTS

The work in this report was conducted and coordinated by a fuels characterization subgroup of CRC's Fuels for Advanced Combustion Engines (FACE) Working Group of the Advanced Vehicle, Fuel, and Lubricants (AVFL) Committee. Members of the working team included: Bill Cannella, Michael Foster, Garry Gunter, Bill Leppard, John Orban and Ken Wright.

Following the successful development of the CRC FACE Diesel Fuels, Ken Wright and Bill Leppard initiated efforts to design a matrix of reference gasoline fuels, which are denoted as the CRC FACE Gasolines. Bill Leppard and John Orban used fuels blending models and statistical techniques to generate a matrix of candidate fuel formulations that were ultimately down-selected to 10 formulations. Ken Wright, Garry Gunter, Michael Foster, and Bill Cannella arranged for the fuels' properties and compositions to be characterized in their company laboratories. In addition, CRC provided funds for the fuels to be analyzed by a contract laboratory.

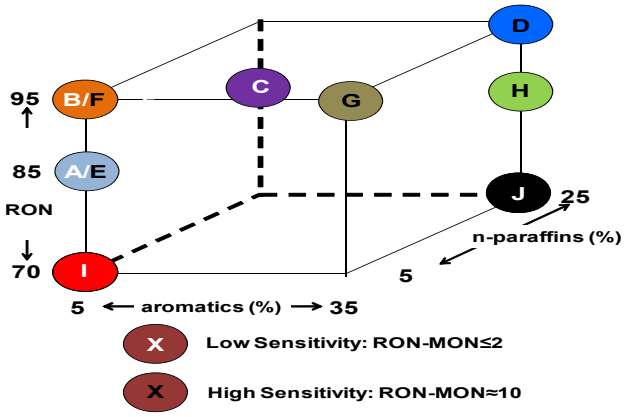
EXECUTIVE SUMMARY

This report provides detailed results from a variety of standard ASTM International-type analyses and advanced characterization techniques conducted to measure the chemical and physical properties of a matrix of gasoline test fuels known as the Fuels for Advanced Combustion Engines (FACE) Gasolines. In addition, results are reported from analyses conducted on blends of ethanol at levels of 10, 15, and 30 volume % (vol.%) with four of the FACE gasolines.

The work was coordinated by a subgroup of the Coordinating Research Council's (CRC's) Advanced Vehicle, Fuel, and Lubricants Committee's FACE Working Group. It parallels and complements the work done previously on the FACE Diesel Fuel matrix.

The FACE Gasoline matrix consists of 10 fuels designed around 4 properties of primary importance to the performance of advanced gasoline-fueled engines: Research Octane Number (RON); Octane Sensitivity (S=RON-MON); aromatics content; and normal-paraffin (n-paraffin) content. The RON and S parameters are measures of a fuel's autoignition quality while the aromatics and n-paraffin content are measures of a fuel's composition. The fuel target levels selected were: RONs of 70, 85, and 95; "low" and "high" octane sensitivities of ≤2 and ~ 10, respectively; aromatics contents of 5 and 35 vol.%; and n-paraffin contents of 5 and 25 vol.%. It was recognized that some of these targets are conflicting (i.e high aromatics content with low octane sensitivity) and that required trade-offs would result in some of the target parameters not being completely met for some fuels.

A full-factorial set of test gasolines with these target levels would consist of 24 fuels. Statistical techniques (described in this report) were used to reduce this to a tractable number of 10 fuels, while still maintaining a statistically sound matrix, which is shown in the Figure below. Although the RON values of 70 and 85 and the octane sensitivity of 2 are lower and n-paraffin content of 25 vol.% are higher than currently found in market gasolines, they appear to be potentially relevant for emerging advanced low temperature combustion engines and so were included in this matrix of research fuels. The CRC FACE Working Group designed this matrix of research fuels. A commercial vendor (Chevron Phillips Chemical Co. – CPChem) has produced and made the fuels available for purchase in research quantities to engine and advanced combustion researchers to enable consistent comparisons of results from different laboratories and test platforms based on the same set of fuels.



In addition to designing the gasolines, a key goal of the current project was to characterize as fully as possible the chemical and physical properties of the FACE Gasolines and selected blends with ethanol and to make that information available to the engine and advanced combustion research and development (R&D) communities to enable selection of standardized test fuels for their programs and correlation of test results to fuel composition and properties.

In support of this project, standard ASTM tests were conducted at several different laboratories to measure the following properties: Research Octane Number (RON); Motor Octane Number (MON); API gravity; density; RVP; distillation profile; net heat of combustion; elemental carbon, hydrogen, and sulfur; and fuel composition. The fuel composition analytical methods consisted of fluorescent indicator adsorption (FIA), supercritical fluid chromatography (SFC), and detailed hydrocarbon analyses (DHA) by one-dimensional gas chromatography with a flame ionization detector (1D GC-FID). Results of those analyses indicate the following.

- As expected, conflicts in the target properties for some of the fuels (such as high aromatics level coupled with low octane sensitivity) led to some trade-offs that resulted in some deviation in the actual properties from the design properties.
- The RON values come close to meeting the targets for most of the fuels. Fuels E, H, and J have values that are 2.4-3.8 units higher than the targets.
- Three of the four "high" sensitivity fuels have measured values of 5.9-7.1 that are lower than the target value of 10. Two of the "low" sensitivity fuels have measured values (3.4-3.7) that are a bit higher than the target value of ≤2. One of the low sensitivity design fuels ("D") has a value of 7.2 that actually effectively makes it a high sensitivity fuel.
- Detailed hydrocarbon analyses (DHA) indicate that the n-paraffins contents range from 22.5-31.6 vol.% for the four FACE Gasolines that had targets of 25 vol.% and from 4.4-11.7 vol.% for the six FACE Gasolines that had targets of 5 vol.%.
- DHAs indicate that the aromatics contents range from 31.7-35.8 vol.% for the four FACE Gasolines that had a target of 35 vol.% and 0-10.9 vol.% for the other fuels that had a target of 5 vol.%
- The high sensitivity fuels contained the high sensitivity components of naphthenes (10.5-20.8 vol.%) and olefins (6.8-12.7 vol.%). The exception was Gasoline "D" which had neither of these components, but whose high sensitivity was derived from aromatics components.
- Five of the FACE Gasolines ("A", "B", "C", "F" and "I") are very rich in isoparaffins with contents ≥ 67.6 vol.%.
- For the four FACE Gasolines blended with ethanol, RON continues to increase as the ethanol levels increase to 30 vol.%, although the rate of increase lessens as ethanol increases. FACE Gasoline B which has the highest RON of 96, has the highest RON at all ethanol levels, with a value of about 106 at 30 vol.% ethanol. At the same ethanol level, FACE Gasolines A and C have essentially the same RON values. FACE Gasoline H starts with a higher RON value than those of A or C, but has a lower value at ethanol blend levels of 15 and 30 vol.%.

- MON increased as ethanol level increased for FACE Gasolines A, C, and H. However, although the MON value was highest for the blends with FACE Gasoline B, the MON values of those blends were essentially constant.
- For all blends, octane sensitivity increased as ethanol content increased, with the highest values of 12-13 for 30% ethanol blends with FACE Gasolines B and H.
- The D86 distillation curve trends are similar for the four FACE Gasolines. For a given gasoline, all blends start at the same point. At around 10 vol.% distilled, the curves for the ethanol blends diverge from and are lower than the curves for the base gasolines. At a certain point, the distillation curves for the blends rise quickly and re-join the curve for the parent base fuel. The distillation curves for the 30 vol.% ethanol blends are generally flat as a function of increasing vol.% distilled and only start to increase again at about 70-80 vol.% distilled when most of the ethanol has distilled from the liquid.
- The Reid Vapor Pressures (RVPs) peak at about 10-15 vol.% ethanol.

We recommend that engine and combustion researchers use these well-characterized FACE Gasolines in their test programs to enable comparison of results from different laboratories and test platforms. In addition, we recommend that researchers characterize as fully as possible the chemical and physical properties of other fuels that they test so that more robust correlations can be developed between fuel properties and engine and combustion performance.

1. INTRODUCTION

This report summarizes the efforts to design a matrix of gasoline test fuels known as the Coordinating Research Council's (CRC) Fuels for Advanced Combustion Engines (FACE) Gasolines and to extensively characterize the physical and chemical properties of those fuels using standard ASTM International-type analyses and advanced characterization techniques. It also provides information about the properties of 4 of the gasolines blended with 10, 15, and 30 vol.% ethanol.

The FACE Gasolines were designed based on statistical methods and target values established by the CRC Advanced Vehicle, Fuel, and Lubricant (AVFL) Committee's FACE Working Group. A key aspect of the mission of the FACE Working Group is to design sets of test fuels well-suited for research so that researchers evaluating advanced combustion systems can compare results from different laboratories using the same sets of fuels for consistency. The current work on the FACE Gasolines follows on the group's previous success with the FACE Diesel Fuels (1, 2, 3).

The FACE Working Group determined that 4 gasoline properties would be of primary importance to the performance of advanced gasoline-fueled engines: Research Octane Number (RON); Octane Sensitivity (S=RON-MON); aromatics content; and normal-paraffin (n-paraffin) content. The RON and S parameters are measures of the fuel autoignition quality while the aromatics and n-paraffin content parameters are measures of the fuel chemistry. Since it was expected that some users would want to investigate some fuels without ethanol, the decision was made to exclude ethanol from the base fuel set. The fuel target levels selected were: RONs of 70, 85, and 95; "low" and "high" octane sensitivities of ≤2 and ~ 10, respectively; aromatics contents of 5 and 35 vol.%; and n-paraffin contents of 5 and 25 vol.%. A full-factorial set of test gasolines with these target levels would consist of 24 fuels. Statistical techniques (described in the next section) were used to reduce this to a tractable number of 10 fuels, while still maintaining a statistically sound matrix. The FACE Gasolines design matrix is depicted in Figure 1:

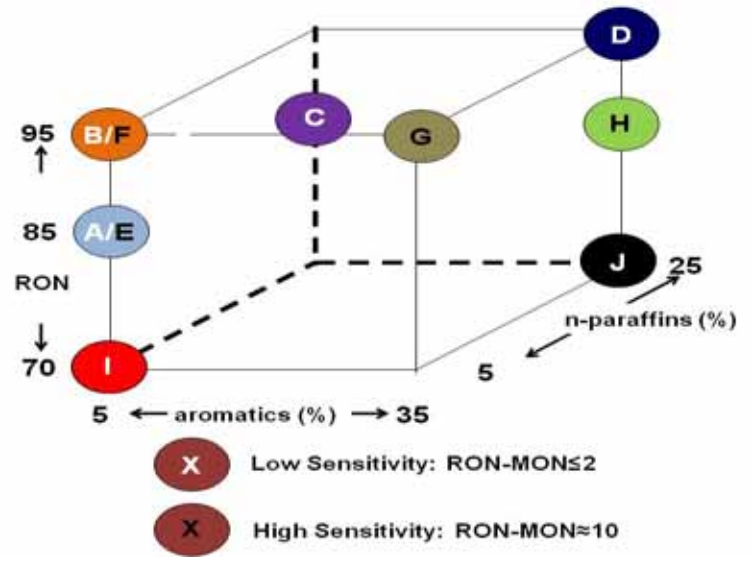


Figure 1: FACE Gasolines Design Matrix

Although the target RON values of 70 and 85 and the octane sensitivity of 2 are lower and n-paraffin content of 25 vol.% are higher than currently found in market gasolines, they appear to be potentially relevant for emerging advanced low temperature combustion engines and so were included in this matrix of research fuels.

A commercial fuels blender (Chevron Phillips Chemical Co. – CPChem) agreed to work with the FACE Working Group and provide blend formulation candidates for each of the target fuels and to manufacture and make available for sale drum quantities of the final formulations. The FACE Working Group directed that the fuel blends should consist of refinery blending streams to the maximum possible extent, but would allow a maximum of five pure compounds to be added with a maximum concentration of 10 vol.%. Also, the olefin content was limited to a maximum of 10 vol.% and for safety reasons the Reid Vapor Pressure was set at a minimum of around 7 psi. The suggested variations in the concentrations of the aromatics and n-paraffins were ±2 vol.%. The suggested variations in the RON and octane sensitivity were ± 2 octane numbers. It was recognized that some of the target fuel properties would lead to conflicts for some fuels (i.e. high aromatics content, but low sensitivity for fuel "D"), and that some trade-offs would be required leading to some of the targets not being completely met.

As soon as CPChem's manufacturing of the commercial batches was completed, a subgroup of the FACE Working Group set about to characterize as fully as possible the chemical and physical properties of the FACE Gasolines and to make that information available to the advanced combustion research and development (R&D) community to enable selection of standardized test fuels for their programs and correlation of test results to fuel composition and properties. In support of that effort, standard ASTM tests were conducted at several different laboratories to measure the following properties: Research Octane Number (RON); Motor Octane Number (MON); API gravity; density; RVP; distillation profile; net heat of combustion; elemental carbon, hydrogen, and sulfur; and fuel composition. The fuel composition methods consisted of fluorescent indicator adsorption (FIA), supercritical fluid chromatography (SFC), and detailed hydrocarbon analyses (DHA) by one-dimensional gas chromatography with a flame ionization detector (1D GC-FID). In general the lab-to-lab variation in these tests was low, less than 1% of the mean. Because of this good agreement in the following charts and text generally the average values are used without error bars. In addition, 5-gallon sized blends of 4 of the FACE Gasolines (A, B, C, and H) with 10, 15, and 30 vol. % ethanol were prepared and also characterized.

This report is organized into the following sections:

- Section 2 provides details on the statistical techniques used to design the FACE Gasolines matrix
- Section 3 contains the results of the analyses of the FACE Gasolines
- Section 4 discusses the results of the analyses of the FACE Gasoline blends with ethanol
- Section 5 presents a summary and conclusions
- Section 6 lists the references cited
- Appendix A provides tables of the properties of the FACE Gasolines
- Appendix B provides tables of the properties of the FACE Gasolines blended with ethanol

2. STATISTICAL DESIGN OF FACE GASOLINES MATRIX

As mentioned in the Introduction, the FACE Gasolines matrix was designed around the following four parameters: RON, octane sensitivity (S), aromatics content, and n-paraffins content. The target levels selected were:

RON: 70, 85, and 95
Sensitivity: ≤2 ("low") and ≈10 ("high")
Aromatics: 5 and 35 vol.%
n-paraffins: 5 and 25 vol.%

A full-factorial set of test gasolines with these target levels consists of the twentyfour fuels listed in Table 2.1. Bill Leppard then used information about the refinery streams and components then available to CPChem, the fuels blender, and their proprietary non-linear octane blending model to develop candidate fuel formulations. Each blending recipe was optimized by manually adjusting the concentrations of the blending components (blending streams and pure components). In parallel, John Orban used the same information about the refinery streams properties to systematically compute all possible candidate fuel formulations using a non-proprietary linear octane blending model. In both modeling efforts the optimum recipes were determined by considering the normalized deviation between the predicted and target properties of RON, sensitivity, aromatics vol.%, and n-paraffin vol.%. Although the two modeling efforts were conducted independently, there were many interactions during the process resulting in a single set of optimum recipes.

CPChem then used these optimum recipes to prepare and analyze hand blends for all twentyfour possible fuels. These measurements are also listed in Table 1. The FACE Working Group realized that this number of fuels was unrealistic from a manufacturing, cost, and testing perspective and decided to limit the total number of fuels to ten

One thing to note from the table is that four of the eight possible 70 RON fuels (designated by a "*" in the table) were not blended because their model-predicted properties were too far removed from the target properties. The FACE Working Group decided to select two of the four 70 RON fuels for the final matrix of ten fuels. These were fuels 1 and 10. Fuel 1 was selected because it contained the lowest amount of aromatics and nearly lowest amount of n-paraffins. Fuel 10 was selected because it contained the highest amounts of aromatics and n-paraffins.

The remaining eight fuels were selected from among the sixteen 85 and 95 RON candidates using the D- and G-optimality efficiencies which are two of the most common statistical techniques for evaluating experimental designs. The D-optimality technique generally produces designs that yield small standard errors for the parameter estimates, small correlations between the parameter estimates, and small standard errors for predicted responses within the design space. The G-optimality technique usually produces similar results.

The use of these statistical techniques to identify the optimum set of fuels requires defining the correlation model relating a measured engine response to the selected fuel parameters. Three linear models were selected which included the following parameters: Model 1 – Response=f(RON, aromatics, n-paraffins, and all 1^{st} order interactions of these three parameters); Model 2 – Response=f(RON, sensitivity, aromatics, n-paraffins, and all 2-factor interactions involving RON); and Model 3 – Response=f(RON, sensitivity, aromatics, n-paraffins, and all 2-factor interactions not involving sensitivity). For all three models the D- and G-optimality efficiencies were calculated for all possible sets of eight fuels and the resulting efficiencies were rank ordered. The rank orderings of the fuel sets

between the D- and G-optimality efficiencies were virtually identical. There were, however, slight differences in the rank orderings among the three correlation models. These results were discussed with the FACE Working Group, which decided to select the optimum fuel set associated with Model 2. The target properties for this fuel set are listed in Table 2.2 along with the final fuel designations.

Once the FACE Working Group decided on the final fuel properties, CPChem initiated efforts to make large batches of the fuels, one at a time, as time and equipment availability permitted. At the start of production of each of the fuels, small hand blends were first made since the compositions of some of the available refinery blendstocks had changed since the original handblends were made during the modeling efforts. For some fuels this required several iterations to come close to meeting the target properties. Analyses of the physical and chemical properties of the final commercial blends are presented in the next section.

Table 2.1
Target and Measured Properties of Hand Blends of Optimized Fuel Blends

Fuel	Target Property				Measured Property			
	Arom. Vol.%	n-Par. Vol.%	RON	Sens.	Arom. Vol.%	n-Par. Vol.%	RON	Sens.
1	5	5	70	2	1.6	9.9	72.7	0.9
4	35	5	70	2	*	*	*	*
7	5	25	70	2	4.2	20.8	66.0	0.3
10	35	25	70	2	26.6	23.1	76.4	4.2
13	5	5	70	10	1.5	12.3	78.9	1.2
16	35	5	70	10	*	*	*	*
19	5	25	70	10	*	*	*	*
22	35	25	70	10	*	*	*	*
2	5	5	85	2	1.3	6.6	86.1	0.7
5	35	5	85	2	26.4	9.3	93.5	7.3
8	5	25	85	2	3.1	24.4	83.5	1.3
11	35	25	85	2	26.2	28.0	84.6	5.5
14	5	5	85	10	8.8	7.4	88.6	6.6
17	35	5	85	10	31.1	13.1	86.3	6.0
20	5	25	85	10	11.2	19.4	85.6	3.2
23	35	25	85	10	33.7	21.0	86.3	7.5
3	5	5	95	2	4.6	8.1	95.3	3.5
6	35	5	95	2	26.2	6.5	98.7	8.6
9	5	25	95	2	12.5	17.2	91.5	3.9
12	35	25	95	2	27.1	19.7	94.0	7.0
15	5	5	95	10	8.7	4.1	94.8	8.6
18	35	5	95	10	31.3	3.7	97.1	10.3
21	5	25	95	10	8.8	14.3	92.4	6.5
24	35	25	95	10	32.5	20.5	91.5	7.7
* - Not blended because model-predicted properties differed too significantly from target properties								

Table 2.2
Target Fuel Parameters for Final Fuel Set

Final FACE Gasoline Designation	Initial Fuel Number	Aromatics Vol.%	n-Paraffins Vol.%	RON	Sensitivity
A	2	5	5	85	Low (≤2)
B	3	5	5	95	Low (≤2)
C	8	5	25	85	Low (≤2)
D	12	35	25	95	Low (≤2)
E	14	5	5	85	High (≈10)
F	15	5	5	95	High (≈10)
G	18	35	5	95	High (≈10)
H	23	35	25	85	High (≈10)
I	1	5	5	70	Low (≤2)
J	10	35	25	70	Low (≤2)

3. ANALYTICAL RESULTS FOR FACE GASOLINES

In this section, results of the analyses of the physical and chemical properties of the first commercial batches of each of the FACE Gasolines are discussed. Chevron, Phillips 66, BP and a contract laboratory conducted the analyses. Also included are the data provided on the CPChem Certificates of Analyses (COAs). Note that future production runs that would be required to remake fuels that sell out likely will result in some changes to the fuel property values reported here for the first production run.

3.1 ASTM TEST RESULTS FOR PHYSICAL PROPERTIES

ASTM methods were used to measure the RON, MON, API gravity, density, distillation profiles, RVP, and net heats of combustion of all of the FACE Gasolines. The results of these analyses are summarized in the sections below and also listed in detail in Table A.1 located in Appendix A.

3.1.1 RON, MON, and Octane Sensitivity

The ignition qualities of gasolines are typically characterized by RON and MON values. RON values were measured in CFR engines per ASTM method D2699 (4). Although the measurements were conducted in several labs, the lab-to-lab reproducibility was very good so only the average values are reported here (but individual values are reported in Table A.1). Bar charts of the average RON values for each fuel are presented in Figure 3.1 (middle bars). Also included are the original design targets (1st bars) and the values reported on the CPChem Certificates of Analysis (COA) (3rd bars). For most fuels, the 3 values are very close to each other (within ±1 unit of each other). The largest differences between measured and target values are for fuels E, H, and J where the measured values are about 2.4-3.8 units higher. Fuel J is also noteworthy because the value measured (1 lab only) is 2 units higher than the CPChem COA.

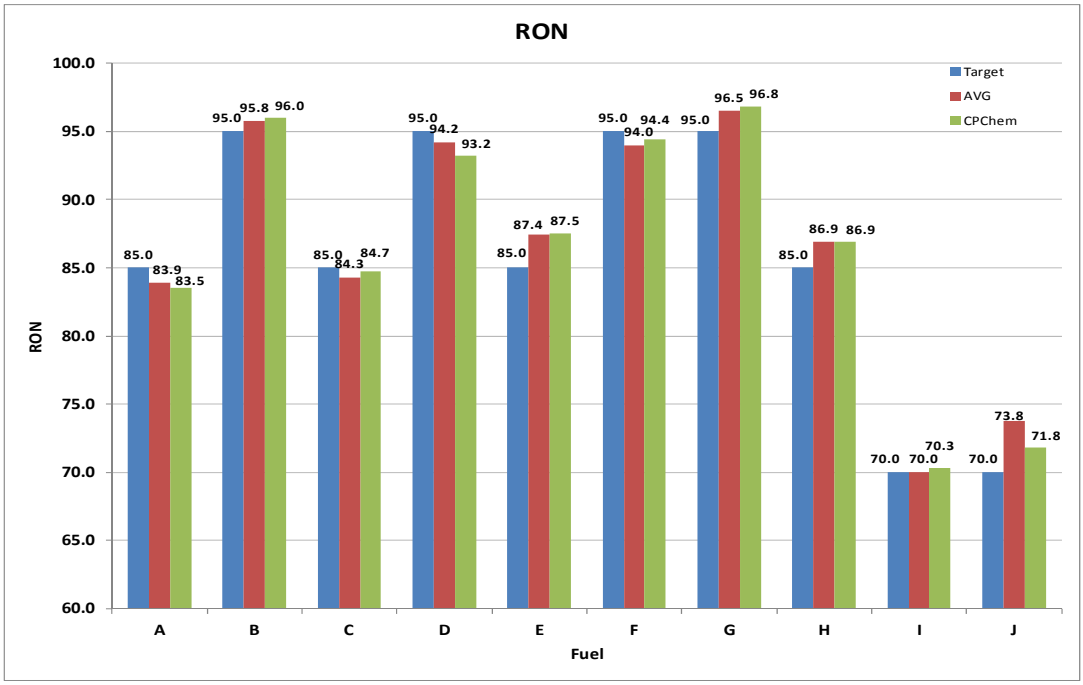


Figure 3.1: RON Values of FACE Gasolines

MON values were measured in CFR engines per ASTM method D2700 (5). Although the measurements were conducted in several labs, the lab-to-lab reproducibility was very good so only the average values are reported here (but individual values are reported in Table A.1). Bar charts of the target, measured, and CPChem COA MON values for each fuel are presented in Figure 3.2. The "target" MON values were determined by subtracting the target octane sensitivities from the target RON values. The largest difference between the values in this project and those reported on CPChem's COA is 1.3 for fuel J. The largest differences between the measured and target values are for fuels D, E, F, and H. For Gasolines E, F, and H the measured values are about 3-6 units higher than target, while for gasoline D, the measured values are about 6 units lower than the target.

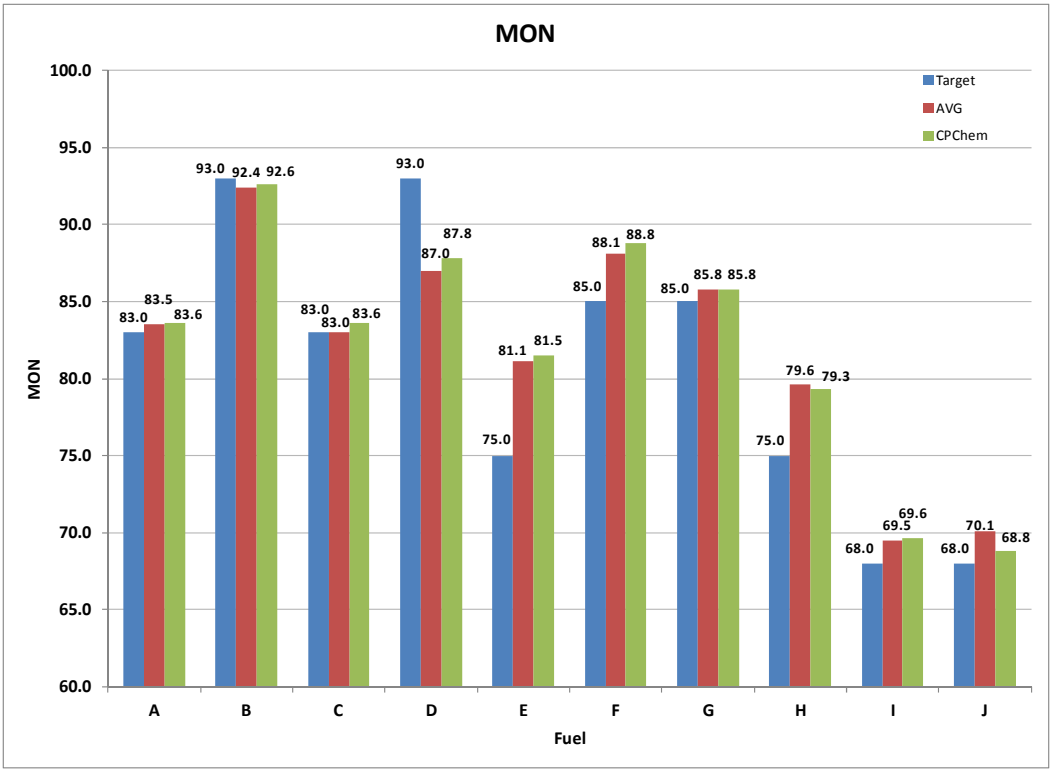


Figure 3.2 MON Values of FACE Gasolines

Octane Sensitivity (S=RON-MON) values are presented in the bar charts in Figure 3.3. The average sensitivities measured by the labs in this project are very close to those reported in CPChem's COAs with the exception of Gasoline D. The measured values for the three of the four high sensitivity fuels are quite a bit lower than the target value of 10, in the range of 5.9-7.1. The exception is Gasoline G, which comes close to meeting the target value. Of the six low sensitivity fuels, three (Gasolines A, C, and I) have values that meet the target value of ≤2, two have values that are slightly higher (Gasolines B and J) and one (Gasoline D) has a value that is significantly higher and in the range of the high sensitivity gasolines. This discrepancy with Gasoline D is not surprising since it is very difficult to produce a low sensitivity fuel with a high level of aromatics, which typically have high sensitivities. Thus relative to the other manufactured FACE Gasolines, Gasoline D should be considered a "high" sensitivity fuel.

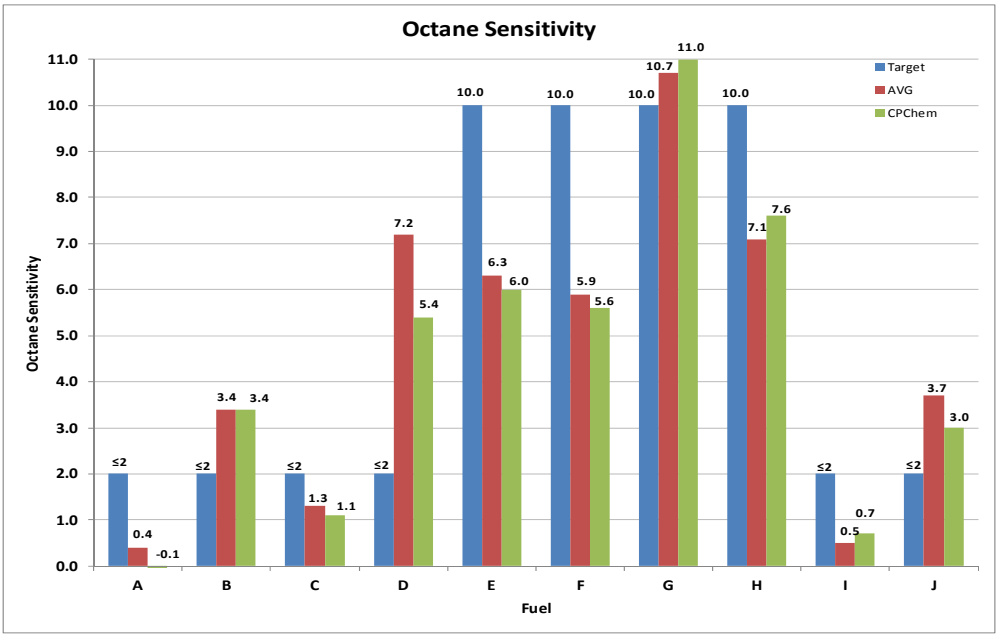


Figure 3.3 Octane Sensitivity Values of FACE Gasolines

3.1.2 Distillation Characteristics

The distillation properties of the fuels were determined by ASTM D86 (6). The D86 values obtained in this study were very close to those reported on CPChem's COAs. The average of those two sources are plotted in Figure 3.4. The values are also tabulated in Table A.1. The temperature corresponding to a given recovery fraction X is designated as TX (i.e., T90 indicates the temperature at which 90% of the fuel has been vaporized and recovered). The initial boiling points (IBP) of all of the fuels are in a relatively narrow range of 90-110˚F. In contrast, the end boiling points (EBP) range from 253-410˚F. Gasolines E, G, and H, which are three of the four high sensitivity fuels, have the highest EBPs. Gasoline E has a relatively steep increase in temperature of 140˚F from T90-EBP. Gasolines I and A, the two fuels having low sensitivity, aromatics, and n-paraffin and low-mid RON, have the lowest EBPs. Gasoline I also has a relatively flat distillation profile from T30-T90.

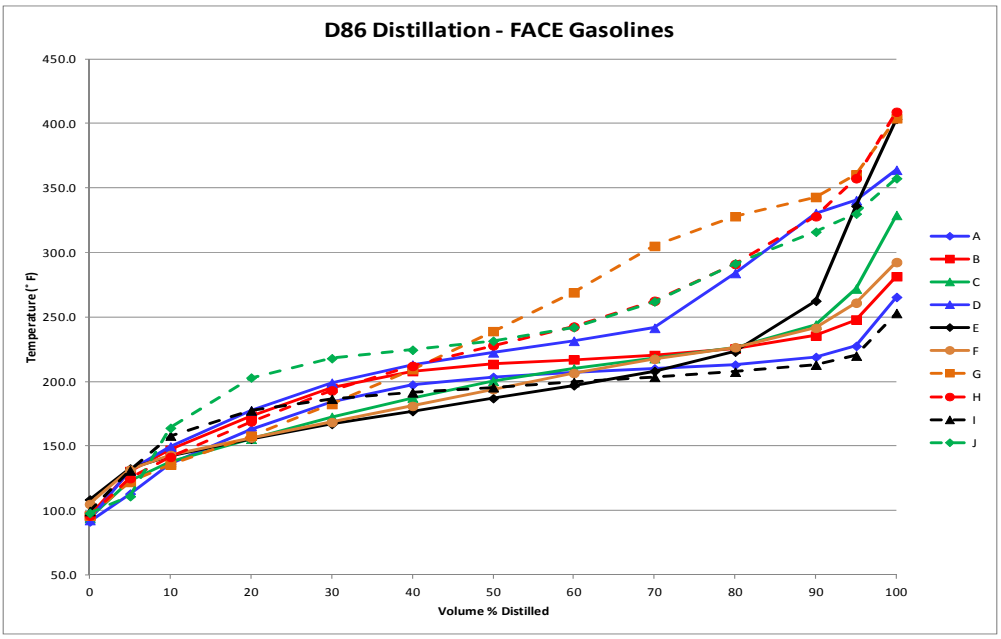


Figure 3.4 ASTM D86 Distillation Curves for the FACE Gasolines

3.1.3 Reid Vapor Pressure (RVP)

The RVPs were determined using ASTM method D5191 (7). The values measured in this project were in excellent agreement with those reported by CPChem COAs (within 0.1 psi). The averages of both values are depicted in the bar charts in Figure 3.5. The values range from 6.7 to 8.05 psi.

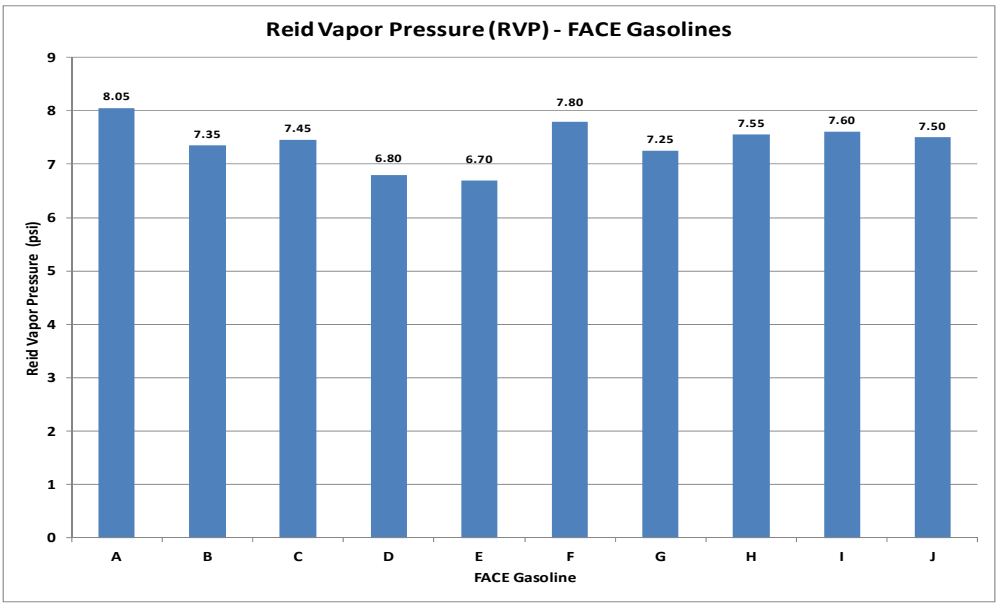


Figure 3.5 Reid Vapor Pressures of FACE Gasolines

3.1.4 API Gravity and Density

The API gravities and densities of the fuels were measured using ASTM method D4052 (8). The agreement between the values measured in this project and the values reported in the CPChem COAs. The individual values are listed in the Summary Table A.1 in Appendix A. The average of both values are plotted in the bar charts in Figures 3.6 and 3.7 for API Gravity and density, respectively. As expected, the FACE Gasolines (D, G, H, and J) having the highest aromatics content have the lowest API Gravities and highest densities.

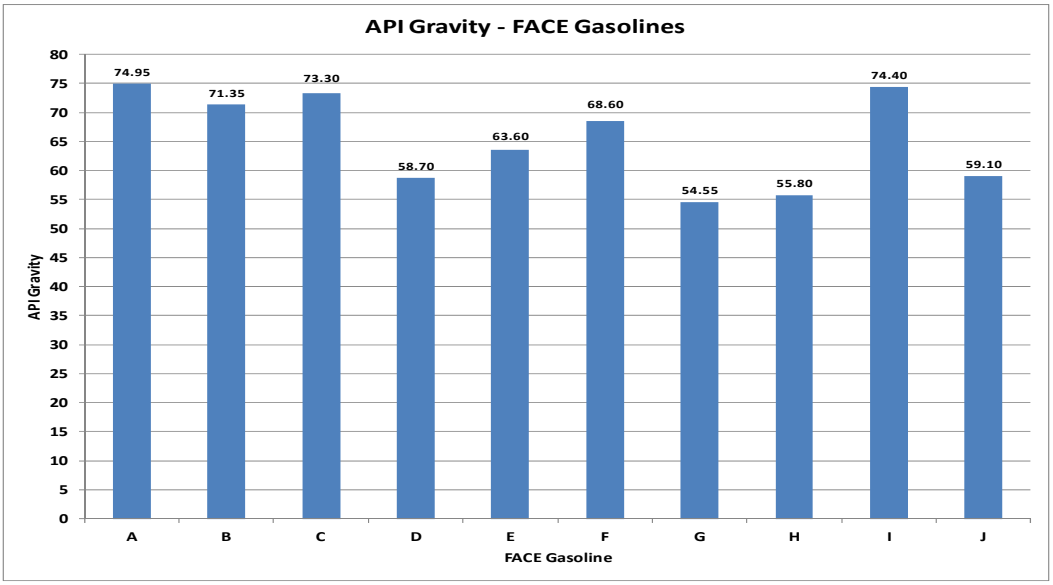


Figure 3.6 API Gravities of FACE Gasolines

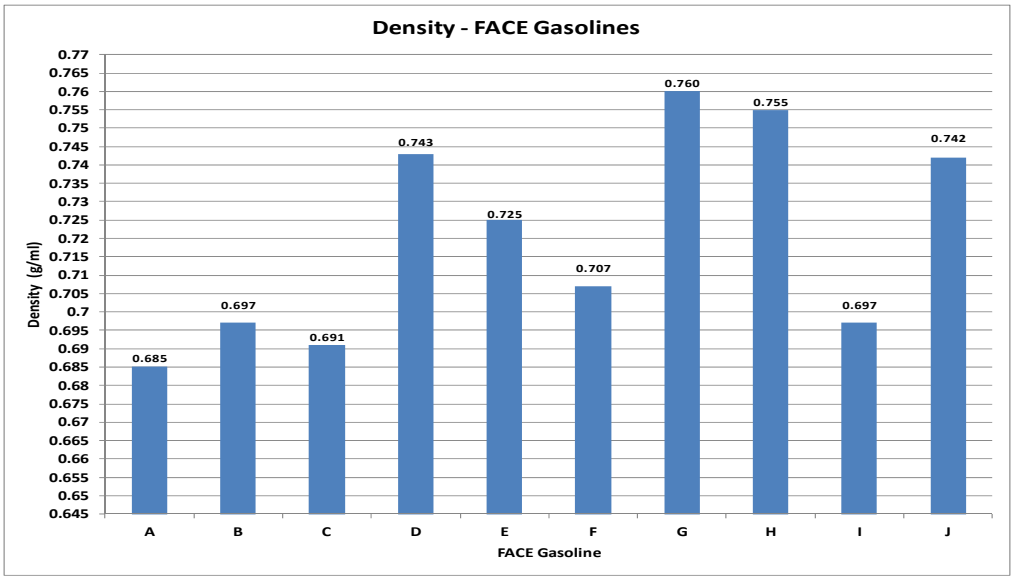


Figure 3.7 Densities of FACE Gasolines

3.1.5 Net Heat of Combustion (NHC)

Net Heats of Combustion were measured using ASTM method D240 (9). The values are depicted in the bar charts in Figure 3.8. In addition, for two of the FACE Gasolines (C and J), the values were also measured using ASTM method D4809 (10). The D4809 values were very close to those obtained from method D240 (within 100 BTU/lb). TheD240 values range from 18602 to 19251 BTU/lb. As expected, the FACE Gasolines having the highest aromatics content (D, G, H, and J) have the lowest net heat of combustion. The FACE Gasolines having saturates content >90% (A, B, C, and I) have the highest net heat of combustion.

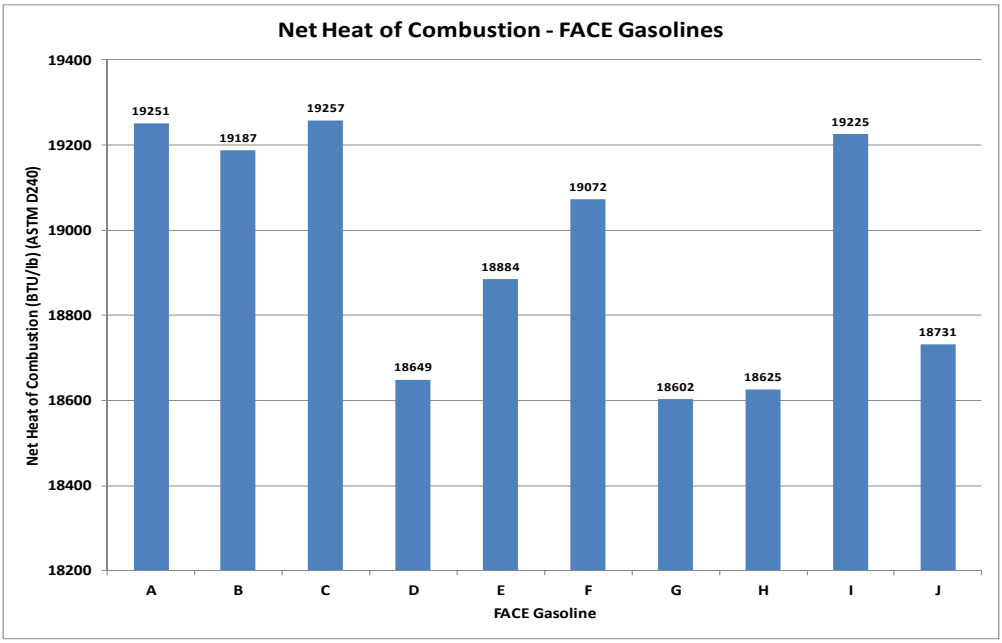


Figure 3.8 ASTM D240 Net Heats of Combustion of FACE Gasolines

3.2 CHEMICAL PROPERTIES OF FACE GASOLINES

The various types of hydrocarbons in the fuels were characterized by several techniques, including: supercritical fluid chromatography (SFC) and detailed hydrocarbon analysis (DHA) by gas chromatography using a flame ionization detector (GC-FID). In addition, the carbon, hydrogen, and sulfur contents were measured. Results are reported in the following sections.

3.2.1 Aromatics by Supercritical Fluid Chromatography (SFC)

The SFC method of ASTM D5186 (11) separates the hydrocarbons into three fractions: monoaromatics, polyaromatics, and non-aromatics and characterizes the composition in terms of mass %. Bar graphs of the results are presented in Figure 3.9. Samples of FACE Gasolines B, D, E, G, and H were analyzed by two labs. The results from the two labs were very close to each other and so the averages are depicted in the figure. FACE Gasolines A, B, C, and I have nonromatics levels >90 wt.%. FACE Gasolines D, G, and H have the highest amounts of monoaromatics with values ranging from 39.4-42.0 wt.%. FACE Gasolines E, G, and H appear to have about 1 wt.% polyaromatics.

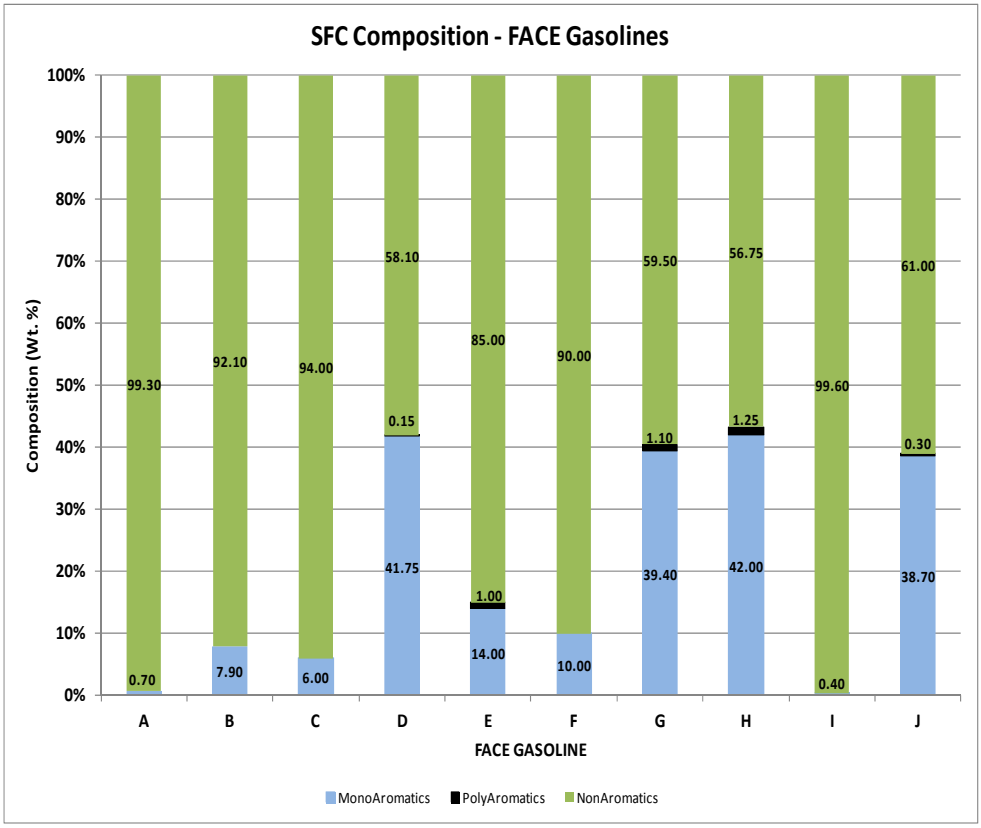


Figure 3.9 Compositions of FACE Gasolines by Supercritical Fluid Chromatography (ASTM D5186)

3.2.2 Hydrocarbons by Detailed Hydrocarbon Analysis (DHA)

Detailed Hydrocarbon Analyses were performed by two labs using gas chromatography with flame ionization detectors (GC-FID). This technique enables the determination of concentration on a species-by-species basis, provided that retention factors have been determined for each species in the fuel. The results from both labs were very close to each other. Bubble charts of the average concentration values (in volume %) are depicted in Figure 3.10 for the low sensitivity fuels and Figure 3.11 for the high sensitivity fuels on a carbon number basis for the five hydrocarbon classes: n-paraffins, iso-paraffins, naphthenes, aromatics, and olefins.

In general, the low sensitivity FACE Gasolines are characterized by large amounts of low sensitivity components such as n-paraffins and iso-paraffins. The high sensitivity FACE Gasolines contain more high sensitivity components such as olefins and naphthenes than the low sensitivity fuels.

The total concentration of components within each of the five hydrocarbon classes were added and the sums are reported in the bar charts in Figure 3.12. The n-paraffin levels range from 22.5-31.6 vol.% for the four FACE Gasolines (C, D, H, and J) that had targets of 25 vol.%. For the other FACE Gasolines that had a target level of 5 vol.%, the n-paraffins levels range from 4.4-11.7 vol.%. The aromatics levels range from 31.7-35.8 vol.% for the four FACE Gasolines (D, G, H, and J) that had targets of 35 vol.%. For the other six FACE Gasolines that had a target level of 5 vol.%, the aromatics levels range from 0-10.9 vol.%. The C_7 aromatic is toluene; the C_8 aromatics consist of a mix of ethylbenzene and the xylene isomers; the C_9 aromatics consist of a mix of trimethylbenzenes and methylethylbenzenes; and the C_{10} aromatics consist of a mix of tetramethylbenzenes, dimethylethylbenzenes, and methylpropylbenzenes. FACE Gasoline E, a high sensitivity fuel, has a naphthene content of 20.8 vol.%, mainly cyclopentane and cyclohexane. Three other high sensitivity fuels (F, G, and H) have naphthenes concentrations of about 11 vol.%, mainly cyclopentane. Those high sensitivity fuels also have the highest olefins content with concentrations ranging from 6.8-12.7 vol.%. FACE Gasoline I also has 6.4 vol.% olefins. The C_6 olefin is 1-hexene. The C_5 olefins consist of a mix of 2-pentene and methyl butenes. In contrast to the high sensitivity fuels, Gasoline D, which was designed to be low sensitivity, but ended up in the high sensitivity range, has essentially no naphthenes or olefins. Its high sensitivity is derived from its high aromatics content.

The C_5 isoparaffin in all of the fuels is 2-methylbutane. The C_6 isoparaffins consist of a mix of 2- and 3-methyl pentanes and 2,3 dimethyl butane. The C_7 isoparaffins in most of the FACE Gasolines consist of a mix of 2- and 3-methyl hexanes and 2,3- and 2,4-dimethylpentanes. The C_8 isoparaffins are predominantly trimethylpentanes, with more than 50% of those being isooctane (2,2,4 trimethylpentane). The other isomers are mainly 2,4- and 2,5 dimethylhexanes and 2-methyl, 3-ethyl pentane.

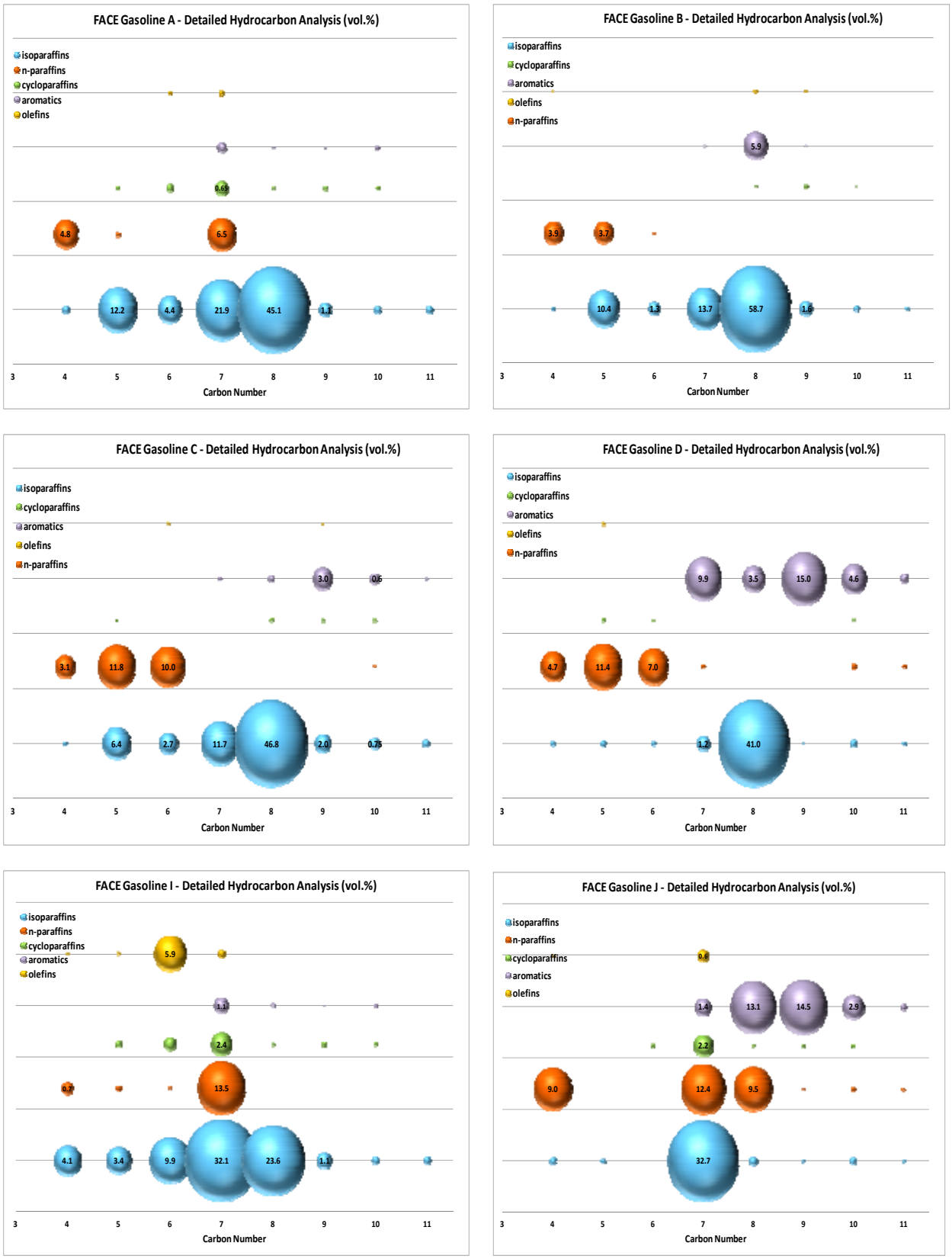


Figure 3.10 Detailed Hydrocarbon Analyses of Low Sensitivity FACE Gasolines

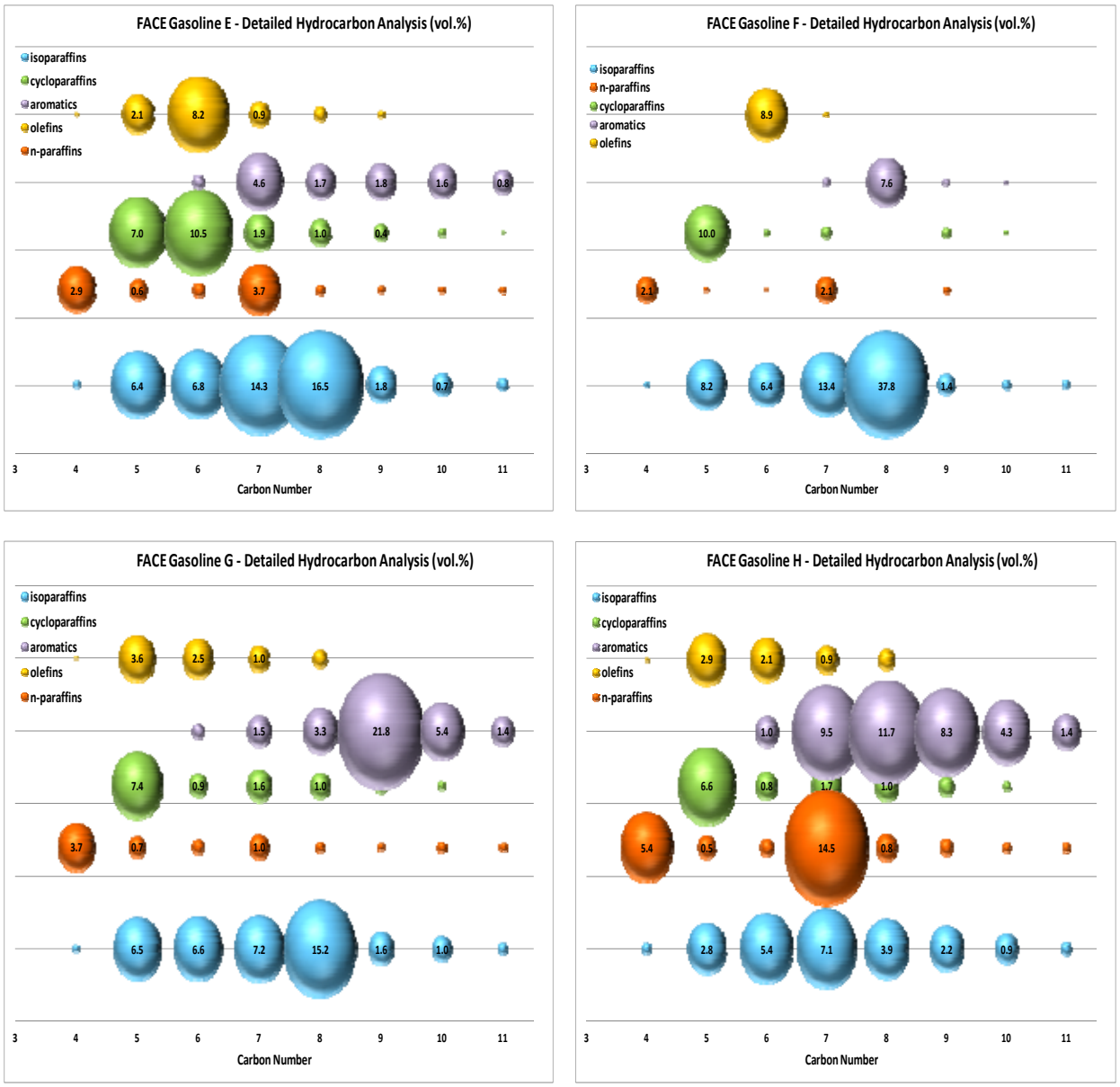


Figure 3.11 Detailed Hydrocarbon Analyses of High Sensitivity FACE Gasolines

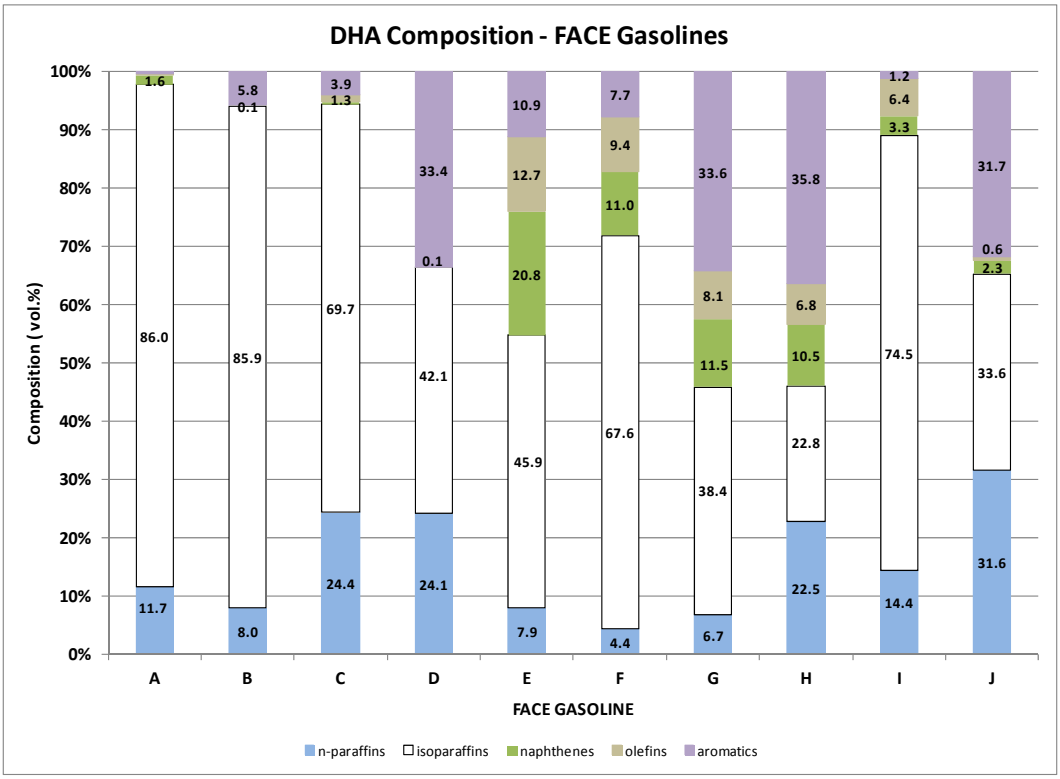


Figure 3.12 Detailed Hydrocarbon Analyses Comparisons of FACE Gasolines

A comparison of the composition results from the DHA and SFC methods is presented in Figure 3.13 for the low sensitivity fuels and Figure 3.14 for the high sensitivity fuels. Also included are Fluorescent Indicator Absorption (FIA – ASTM D1319 (12)) composition results reported on the CPChem COAs. Since the FIA method determines total saturates, the DHA results for n-paraffins, iso-paraffins, and naphthenes must be added together to enable the comparison between those two methods. Similarly since the SFC method directly measures aromatics and total non-aromatics are determined by difference, the olefins amount must be added to the total saturate levels from FIA and DHA to enable comparisons with the non-aromatics values from SFC. The appropriate comparison categories are indicated by dashed lines in Figures 3.13 and 3.14. Of the three methods, SFC generally gives the highest level of aromatics and FIA the lowest. The DHA aromatics values are closer to the FIA levels than to the SFC levels. The DHA olefins are fairly close to the FIA results.

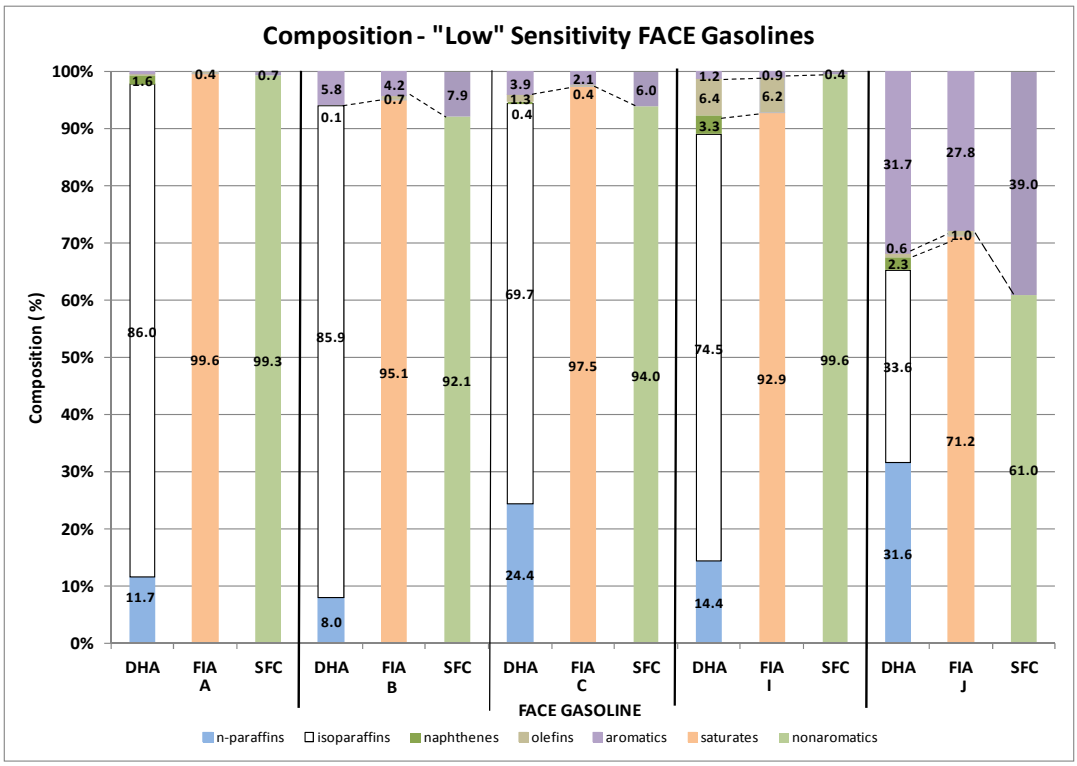


Figure 3.13 Comparison of Composition Methods: FACE Low Sensitivity Gasolines

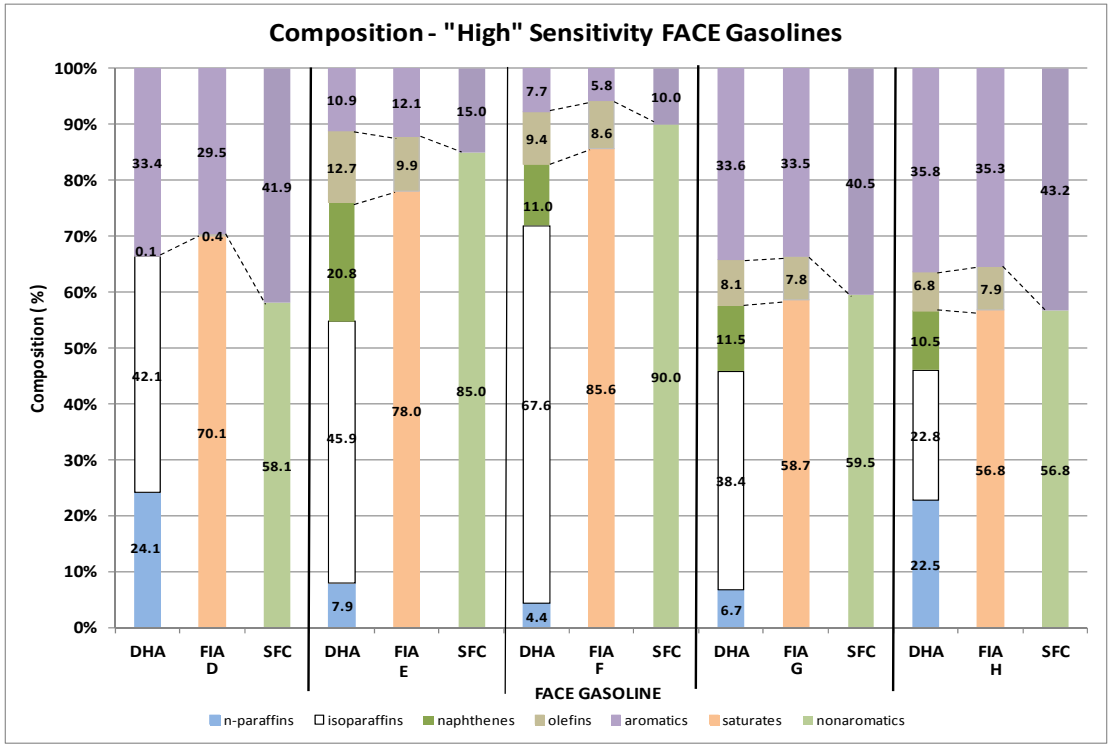


Figure 3.14 Comparison of Composition Methods: FACE High Sensitivity Gasolines

3.2.3 Elemental Analyses

Carbon and hydrogen contents were measured by two labs using ASTM method D5291 (13). The average results are presented in the bar graphs in figure 3.15. The carbon contents range from 83.99-87.48 wt.% and the hydrogen contents range from12.52-16.01 wt.%. As expected, the FACE Gasolines having the highest aromatics content (D, G, H, and J) have the highest carbon and lowest hydrogen contents.

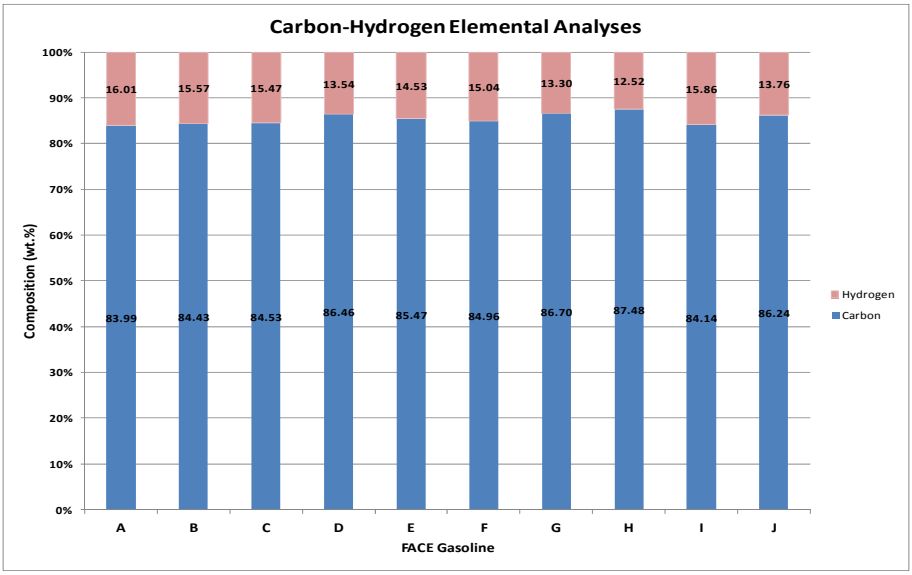


Figure 3.15 Carbon and Hydrogen Elemental Analyses of FACE Gasolines

Sulfur content was measured by one lab ASTM method D5453 (14). The results, displayed in the bar charts in Figure 3.16 are essentially identical to the values reported on the CPChem COAs . All FACE Gasolines had ultra-low sulfur levels. FACE Gasolines E, G, and H had the highest levels at 21, 22, and 15 ppm sulfur. The other fuels had levels ranging from 2-6 ppm.

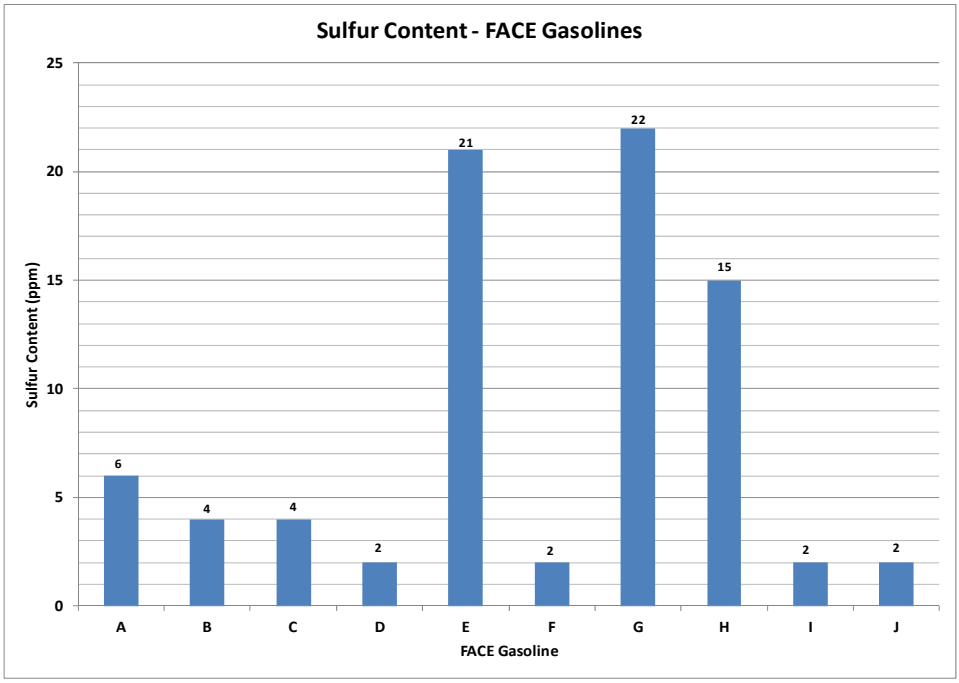
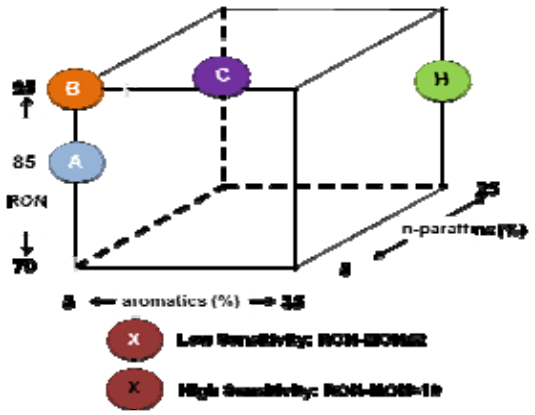


Figure 3.16 Sulfur Levels of FACE Gasolines

4. ANALYTICAL RESULTS FOR FACE GASOLINES BLENDED WITH ETHANOL

Although the FACE Gasolines were not formulated with ethanol, the expectation is that some potential users will be interested in testing the fuels with ethanol added. To assist selection of fuels for those studies, four FACE Gasolines were selected for blending with levels of 10, 15, and 30 vol.% ethanol. The fuels selected for this purpose were: A, B, C, and H. The positions of these fuels in the design matrix are shown below:



In this section, results of the analyses of the ethanol blends are discussed. Chevron, Phillips 66, BP and a contract laboratory conducted the analyses. As mentioned previously, future production runs that are required to remake fuels that sell out likely will results in some changes to the fuel property values reported here.

4.1 ASTM TEST RESULTS

ASTM methods were used to measure the ethanol content, RON, MON, API gravity, density, distillation profiles, RVP, and net heats of combustion of all of the ethanol blends made with the FACE Gasolines. The results of these analyses are summarized below and in Table A.2 located in the Appendix.

4.1.1 Ethanol Content

FACE Gasolines A, B, C, and H were blended with nominally 10, 15, and 30 vol.% ethanol. The concentration of ethanol in each blend were determined using ASTM method D5599 (15) (coupled with ASTM D4052 density measurement) and by detailed hydrocarbon analysis using gas chromatography with a flame ionization detector. The results for both methods were in excellent agreement for all fuels, as shown below in Table 4.1:

Table 4.1
Measured Ethanol Content of FACE Gasoline Blends

	Ethanol Content (vol.%)											
	A			B			C			H		
	10	15	30	10	15	30	10	15	30	10	15	30
D5599	10.1	14.7	29.9	10.0	14.7	30.2	10.2	14.6	29.5	10.2	14.6	30.3
DHA	10.0	14.6	30.1	10.0	14.8	30.1	10.3	14.8	29.9	10.2	14.7	30.4

4.1.2 RON, MON, and Octane Sensitivity

RON values were measured in CFR engines per ASTM method D2699 (4). Although the measurements were conducted in four labs, the lab-to-lab reproducibility was very good so only the average values are reported here (but individual values are reported in Table A.2). Average RON values for each fuel are presented in Figure 4.1. For all four of these FACE Gasolines, the RON values continue to increase even at the 30% ethanol level, although the rates of increase are lower than at lower ethanol levels. FACE Gasoline B, has the highest RON at all ethanol levels, with a value of about 106 at the 30% ethanol level. FACE Gasolines A and C have essentially the same RON values at all ethanol levels, with RON values of about 102 at the 30% ethanol level. FACE Gasoline H without ethanol has a higher RON than A and C, but a lower RON at the 15 and 30% ethanol levels.

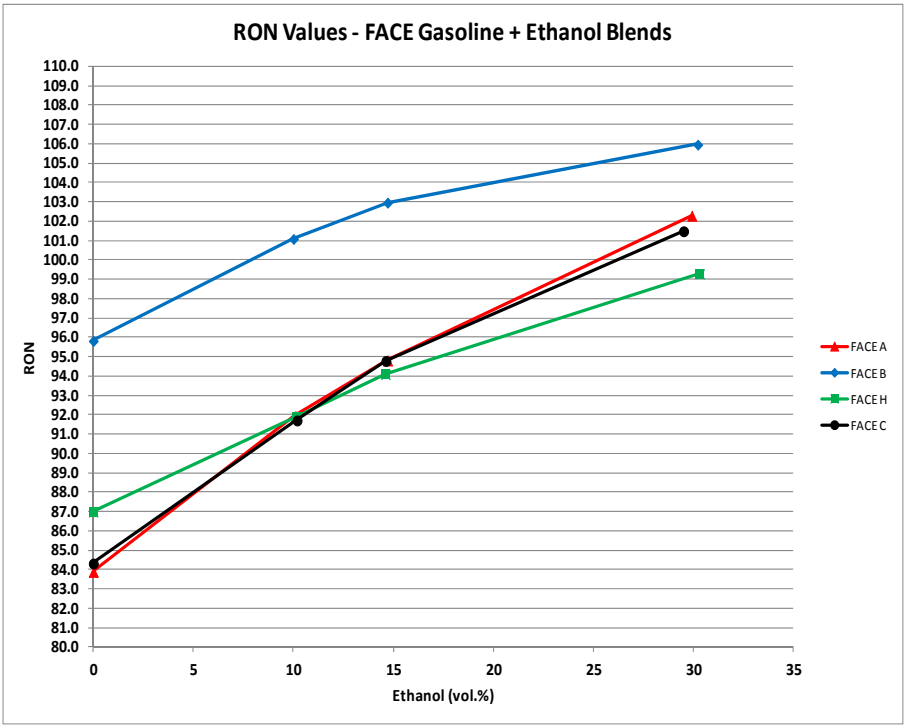


Figure 4.1 RON Values of FACE Gasoline Blends with Ethanol

MON values were measured in CFR engines per ASTM method D2700 (5). Although the measurements were conducted in four labs, the lab-to-lab reproducibility was very good so only the average values are reported here (but individual values are reported in Appendix A.2). The MON values for each fuel are presented in Figure 4.2. FACE Gasoline B has the highest MON values at all ethanol levels, but unlike the other FACE Gasolines, the MON value did not increase with ethanol contents above 10 vol.%. The MON values for FACE Gasolines A and C were essentially the same and higher than those for FACE Gasoline H.

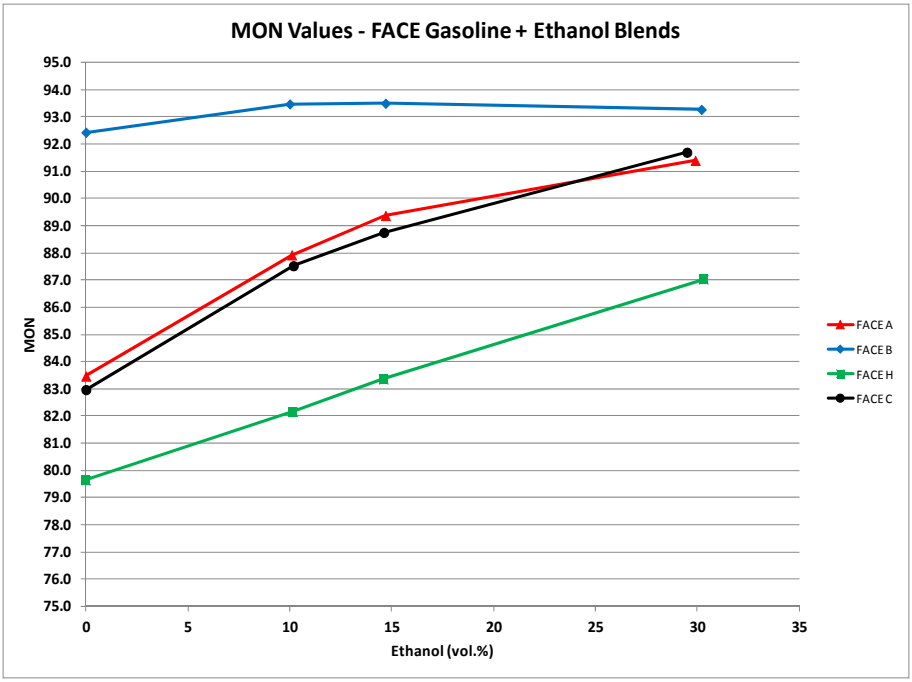


Figure 4.2 MON Values of FACE Gasoline Blends with Ethanol

Octane Sensitivity (S=RON-MON) values are presented in Figure 4.3. As expected due to the relatively high sensitivity of ethanol, the sensitivities of all four FACE Gasolines increase as the ethanol content increases. FACE Gasoline H has the highest sensitivity at all ethanol levels, except at 30 vol.% ethanol where the sensitivity of the FACE Gasoline B blend becomes slightly higher, with values of 12.4 and 13.2, respectively. The sensitivities for FACE Gasolines A and C are very similar to each other, and although lower than the blends for the other FACE Gasolines, have the highest rates of increase at the 30% level.

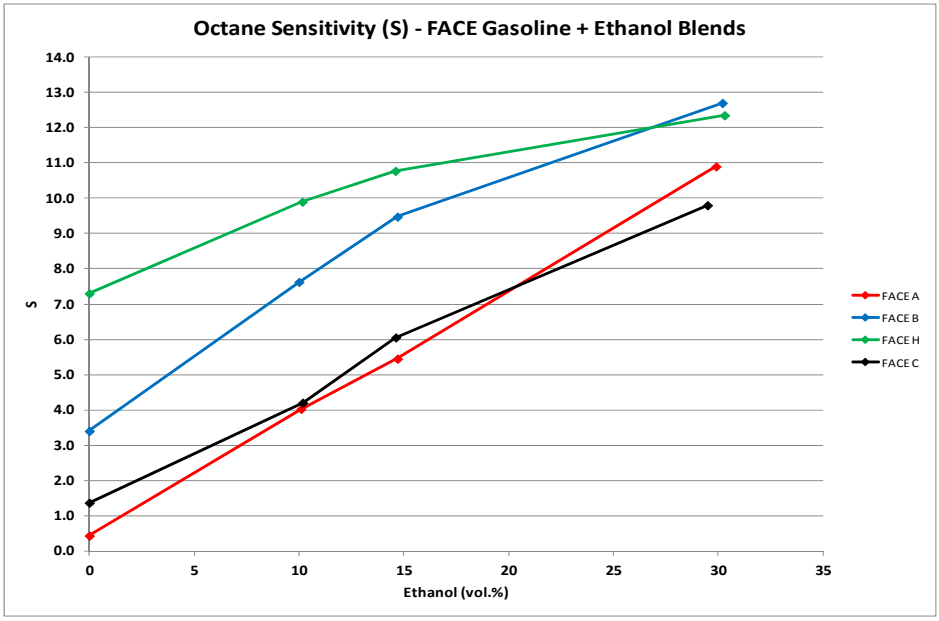


Figure 4.3 Octane Sensitivities FACE Gasoline Blends with Ethanol

4.1.3 Distillation Characteristics

The distillation properties of the fuels were determined by ASTM D86 (6). The values are plotted in Figure 4.4 and tabulated in Table A.2 in the Appendix. The behavior and shapes of the curves are very similar. For a given gasoline, all of the ethanol blends start at about the same IBP. The blends containing ethanol then follow the same curve which is lower than the base gasoline. At a certain point, the ethanol blends then rise quickly to rejoin the distillation curve of the base gasoline. The lower the ethanol content of the blend, the earlier (lower distilled volume %) the curve rejoins the base gasoline curve.

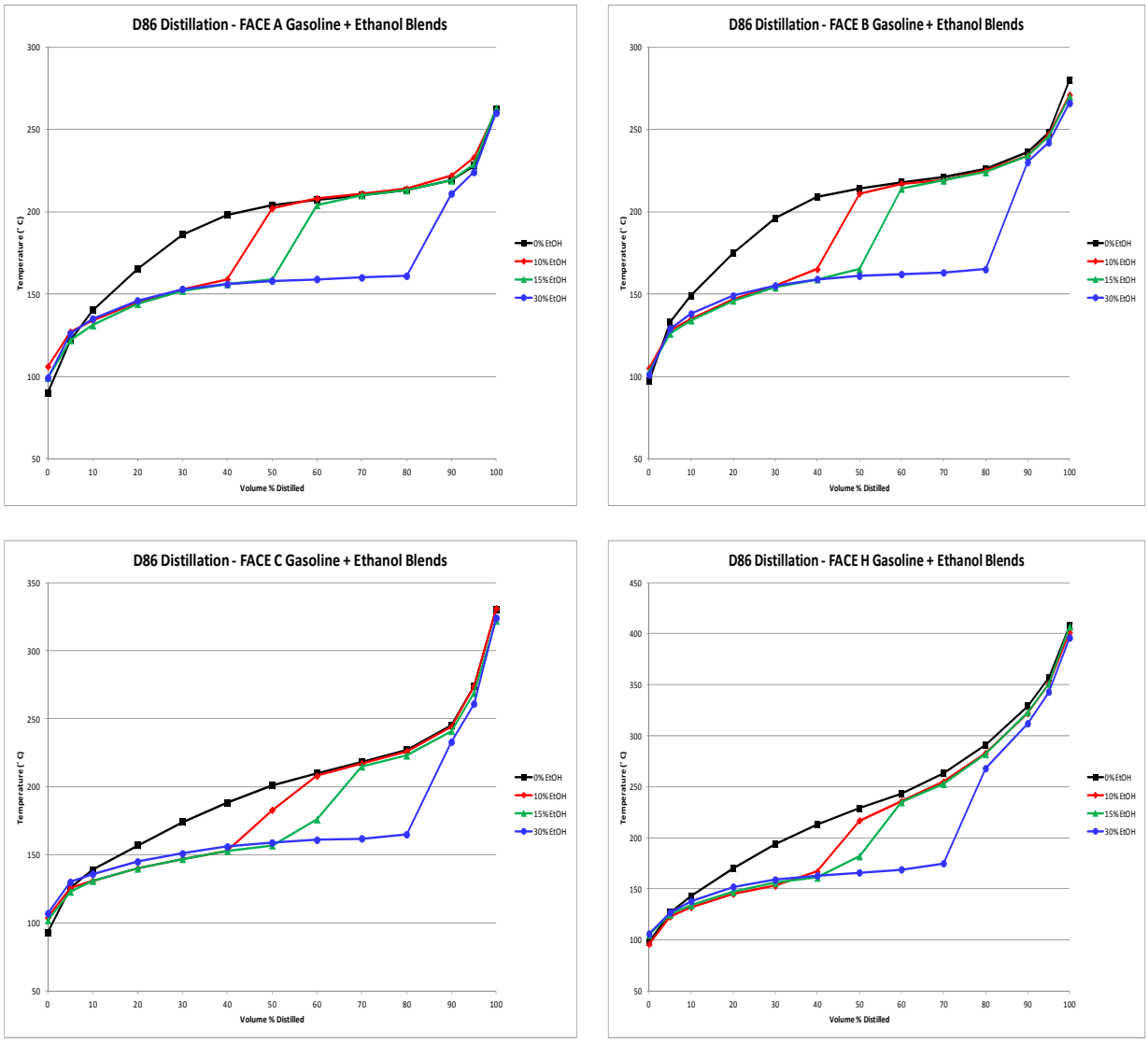


Figure 4.4 ASTM D86 Distillation Profiles for FACE Gasoline Blends with Ethanol

4.1.4 Reid Vapor Pressure (RVP)

The RVPs were determined using ASTM method D5191 (7). The values are plotted in Figure 4.5. For all fuels, the RVP appears to peak between 10 and 15 vol.% ethanol, and then starts to decrease as the ethanol content increases further.

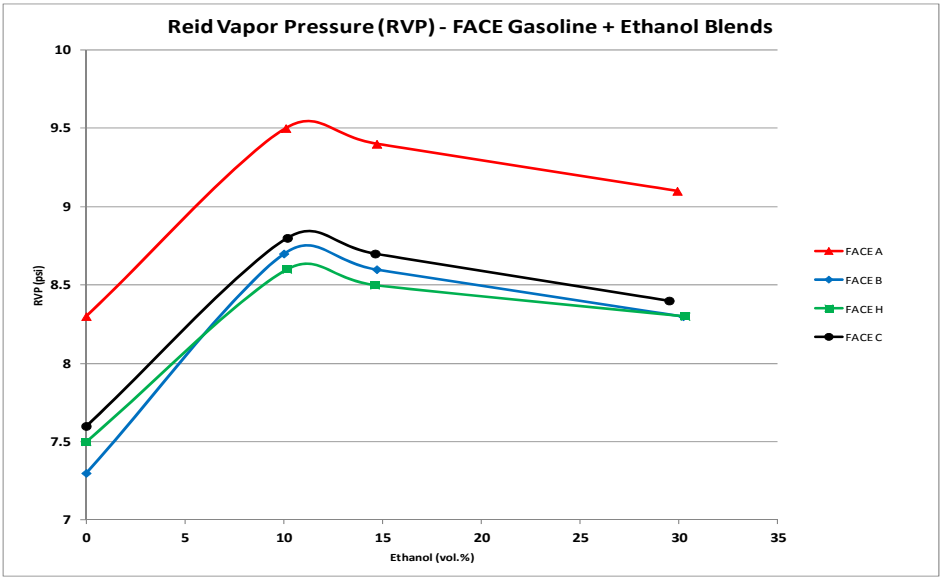


Figure 4.5 Reid Vapor Pressures for FACE Gasoline Blends with Ethanol

4.1.5 API Gravity and Density

The API gravities and densities of the fuels were measured by two labs using ASTM method D4052 (8). The values from the two labs were in excellent agreement and are listed in Table A.2. The average density values are presented in Figure 4.6. For all of the FACE Gasolines, the density increased as the ethanol content increased.

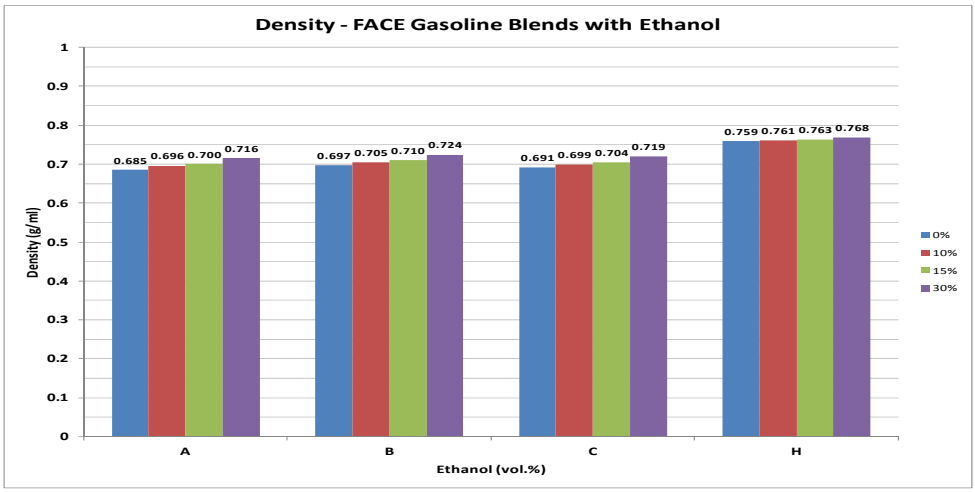


Figure 4.6 Densities of FACE Gasoline Blends with Ethanol

4.1.6 Net Heat of Combustion (NHC)

Net Heats of Combustion were measured by 2 labs using ASTM method D240 (9). For some fuels ASTM method D4809 (10) was also used. The values from both labs and both methods were very close to each other and the average values are plotted in Figure 4.7. As expected, since the net heat of combustion of ethanol is lower than that of gasoline, for all FACE Gasolines the net heat of combustion decreased as ethanol content increased. The decrease appeared to be linear with ethanol content. The decrease appeared to be steepest for FACE Gasoline B.

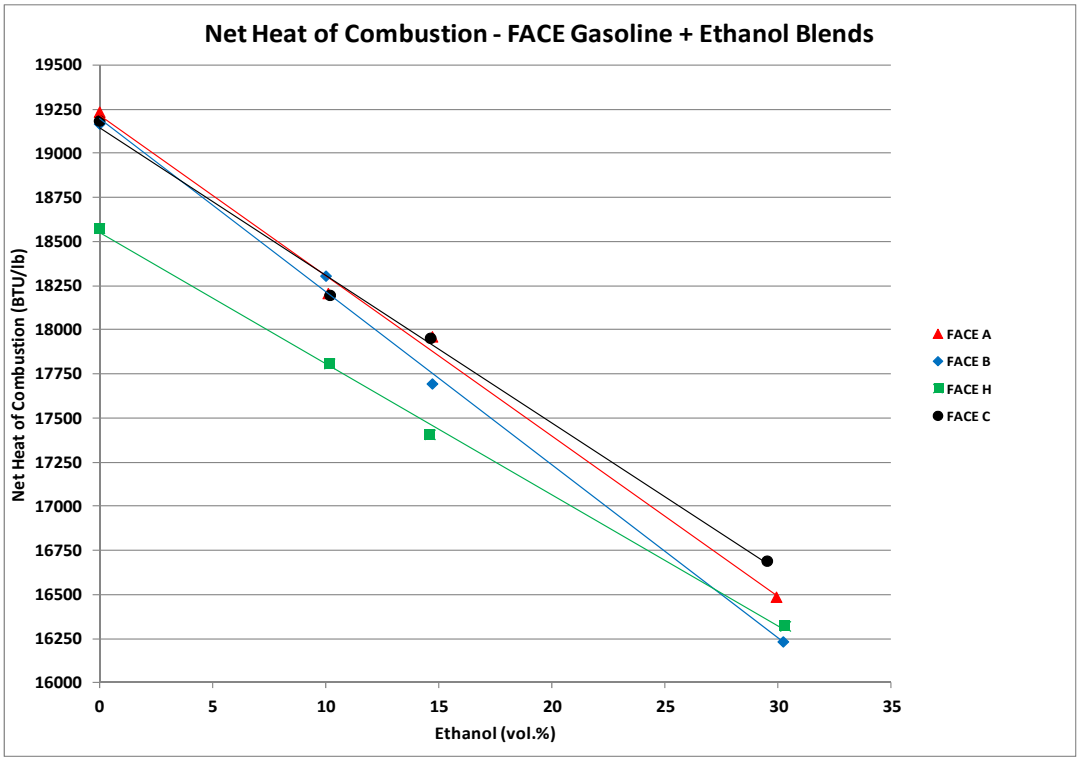


Figure 4.7 Net Heat of Combustion of FACE Gasoline Blends with Ethanol

5. SUMMARY AND CONCLUSIONS

- A subteam of the CRC AVFL FACE Working Group has designed a matrix of reference gasolines known as the FACE Gasolines. A commercial vendor has produced and made the fuels available for purchase in research quantities. It is expected that this will enable consistent comparisons of engine and combustion results from different laboratories and test platforms based on the use of the same set of fuels.
- The matrix is designed around four parameters expected to be of importance for advanced gasoline engines: RON, octane sensitivity, aromatics content, and n-paraffins content.
- Statistical methods were used to identify potential candidate formulations and down-select to a tractable number of 10 formulations.
- Detailed analyses were performed on the physical and chemical properties of the final fuel formulations.
- Generally the property values measured in the current study agreed very well with the values reported on the fuel blender (ChevronPhillips Chemical Company - CPChem) Certificates of Analyses (COAs).
- As expected, conflicts in the target properties for some of the fuels (such as high aromatics level coupled with low octane sensitivity) led to some trade-offs that resulted in some deviation in the actual properties from the design properties.
- The RON values come close to meeting the targets for most of the fuels. Fuels E, H, and J have values that are 2.4-3.8 units higher than the targets.
- Three of the four "high" sensitivity fuels have measured values of 5.9-7.1 that are lower than the target value of 10. Two of the "low" sensitivity fuels have measured values (3.4-3.7) that are a bit higher than the target value of ≤2. One of the low sensitivity design fuels ("D") has a value of 7.2 that actually effectively makes it a high sensitivity fuel.
- Detailed hydrocarbon analyses (DHA) indicate that the n-paraffins contents range from 22.5-31.6 vol.% for the four FACE Gasolines that had targets of 25 vol.% and from 4.4-11.7 vol.% for the six FACE Gasolines that had targets of 5 vol.%.
- DHAs indicate that the aromatics contents range from 31.7-35.8 vol.% for the four FACE Gasolines that had a target of 35 vol.% and 0-10.9 vol.% for the other fuels that had a target of 5 vol.%
- The high sensitivity fuels contained the high sensitivity components of naphthenes (10.5-20.8 vol.%) and olefins (6.8-12.7 vol.%). The exception was Gasoline "D" which had neither of these components, but whose high sensitivity was derived from aromatics components.
- Five of the FACE Gasolines ("A", "B", "C", "F" and "I") are very rich in isoparaffins with contents ≥ 67.6 vol.%.
- Aromatics values determined by SFC were generally higher than the values obtained from DHA. The DHA olefins values were close to the FIA values reported on the CPChem COAs.
- The fuels having the highest aromatics content also have the highest densities and highest net heats of combustion on an energy content per volume basis.
- With regards to distillation properties, for all fuels, the initial boiling points (IBPs) are in a narrow range of 90-110˚F, although the end boiling points (EBPs) range from 253-410˚F. Three

of the high sensitivity fuels have the highest EBPs. The two low-mid RON fuels having low n-paraffins and low aromatics have the lowest EBPs.

- All of the FACE Gasolines have ultra-low levels of sulfur with the highest value at 22 ppm S and most fuels having ≤ 6 ppm S.
- For the four FACE Gasolines blended with ethanol, RON continues to increase as the ethanol levels increase to 30 vol.%, although the rate of increase is lower as the ethanol content increases. FACE Gasoline B which has the highest RON of 96, has the highest RON at all ethanol levels, with a value of about 106 at 30% ethanol. At the same ethanol level, FACE Gasolines A and C have essentially the same RON values. FACE Gasoline H starts with a higher RON value than those of A or C, but has a lower value at blend levels of 15 and 30 vol.%.
- MON increased as the ethanol level increased for FACE Gasolines A, C, and H. The MON values for these fuels were essentially constant even though the highest MON values were found for the ethanol blends with FACE Gasoline B.
- For all blends, octane sensitivity increased as ethanol content increased, with the highest values of 12-13 for 30 vol.% ethanol blends with FACE Gasolines B and H.
- The D86 distillation curve trends are similar for the four FACE Gasolines. For a given gasoline, all blends start at the same point. At around 10 vol.% distilled, the curves for the blends with ethanol diverge from and are lower than the curves for the base gasolines. At a certain point, the distillation curves for the blends rise quickly and re-join the curve for the parent base fuel. The distillation curves for the 30 vol.% ethanol blends are generally flat as a function of increasing vol.% distilled and only start to increase again at about 70-80 vol.% distilled when most of the ethanol has been distilled from the liquid.
- The Reid Vapor Pressures (RVPs) peak at about 10-15 vol.%.
- Densities increase slightly as ethanol increases, while net heats of combustion decrease.

6. REFERENCES

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Appendix A

Properties of FACE Gasolines

Table A.1 Summary Data for FACE Gasolines

Specific Tests: FACE Gasoline:	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**
Research Octane Number (RON) (ASTM D2699):										
-Lab 1	84.3	95.8	85.0	94.6	87.1	94.0	96.9	87.0	70.0	73.8
-Lab 2	83.9	96.0	84.0	93.9	87.7		96.0	86.9		
-Lab 3	83.5	95.7	84.0							
-Average	83.9	95.8	84.3	94.2	87.4	94.0	96.5	86.9	70.15	73.8
-CPChem COA	83.5	96.0	84.7	93.2	87.5	94.4	96.8	86.9	70.3	71.8
Motor Octane Number (MON) (ASTM D2700):										
-Lab 1	83.6	92.3	83.0	87.2	81.3	88.1	85.7	79.7	69.5	70.1
-Lab 2	83.3	93.1	83.0	86.8	80.8		86.0	79.9		
-Lab 3	83.5	91.9	82.9							
-Average	83.5	92.4	83.0	87.0	81.1	88.1	85.8	79.8	69.5	70.1
-CPChem COA	83.6	92.6	83.6	87.8	81.5	88.8	85.8	79.3	69.6	68.8
Sensitivity (RON-MON)										
-Lab 1	0.7	3.5	2.0	7.4	5.8	5.9	11.2	7.3	0.5	3.7
-Lab 2	0.6	2.9	1.0	7.1	6.9		10.0	7.0		
-Lab 3	0	3.8	1.1							
-Average	0.4	3.4	1.3	7.2	6.3	5.9	10.7	7.2	0.5	3.7
-CPChem COA	-0.1	3.4	1.1	5.4	6.0	5.6	11.0	7.6	0.7	3.0
API Gravity (API°) (ASTM D4052):										
-CPChem COA	75.0	71.4	73.4	58.7	63.6	68.6	54.5	56.8	74.4	59.5
-Lab 1	74.9	71.3	73.2	58.7	63.6	68.6	54.6	54.8	74.4	58.7
-Average	74.95	71.35	73.3	58.7	63.6	68.6	54.55	55.8	74.4	59.1
Density (ASTM D4052):										
-CPChem COA			0.691	0.743	0.725	0.707	0.760		0.697	0.741
-Lab 1	0.685	0.697	0.691	0.743	0.725	0.707	0.760	0.759	0.697	0.743
-Average	0.685	0.697	0.691	0.743	0.725	0.707	0.760	0.759	0.697	0.742
RVP (psi) (D5191)										
-CPChem COA	8.1	7.4	7.4	6.8	6.7	7.8	7.2	7.5	7.5	7.5
-Lab 1	8.0	7.3	7.5				7.3	7.6	7.7	
Net Heat of Combustion (BTU/lb) (ASTM D4809):			19186							18680
Net Heat of Combustion (BTU/lb) (ASTM D240):	19251	19187	19257	18649	18884	19072	18602	18625	19225	18731

TableA.1 Summary Data for FACE Gasolines

Specific Tests:	**FACE Gasoline:**	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**
Distillation (˚F) (ASTM D86)											
-CPChem:	IBP	93	95	95	88	110	108	93	94	100	101
	5%	104	128	120	129	131	129	122	123	123	111
	10%	132	145	136	148	142	142	135	140	156	162
	20%	160	172	154	176	155	156	158	168	177	206
	30%	183	194	171	198	166	168	183	192	186	217
	40%	197	207	187	212	177	180	210	211	191	224
	50%	203	213	200	221	186	193	240	227	195	231
	60%	207	216	210	229	197	206	270	242	199	242
	70%	210	220	218	235	208	217	306	262	203	261
	80%	213	225	226	280	222	225	328	291	207	291
	90%	219	235	243	330	267	240	343	327	213	316
	95%	227	248	270	340	343	261	363	358	220	330
	FBP	269	283	328	363	405	294	403	410	259	358
-Lab 1:	IBP	90	97	93	97	107	102	99	98	99	95
	5%	122	133	126	133	134	134	122	127	139	111
	10%	140	149	139	151	143	144	136	143	160	166
	20%	165	175	157	179	156	157	158	170	178	209
	30%	186	196	174	200	168	169	182	194	187	219
	40%	198	209	188	214	177	182	209	213	192	225
	50%	204	214	201	224	188	195	238	229	196	232
	60%	207	218	210	234	197	207	268	243	200	242
	70%	210	221	218	248	208	218	304	263	204	263
	80%	213	226	227	288	224	228	328	291	208	292
	90%	219	236	245	331	258	243	343	329	213	316
	95%	228	248	274	341	329	261	358	357	220	330
	FBP	262	280	330	365	402	291	405	408	247	357
-Average:	IBP	91.5	96	94	92.5	108.5	105	96	96	99.5	98
	5%	113	130.5	123	131	132.5	131.5	122	125	131	111
	10%	136	147	137.5	149.5	142.5	143	135.5	141.5	158	164
	20%	162.5	173.5	155.5	177.5	155.5	156.5	158	169	177.5	203
	30%	184.5	195	172.5	199	167	168.5	182.5	193	186.5	218
	40%	197.5	208	187.5	213	177	181	209.5	212	191.5	224.5
	50%	203.5	213.5	200.5	222.5	187	194	239	228	195.5	231.5
	60%	207	217	210	231.5	197	206.5	269	242.5	199.5	242
	70%	210	220.5	218	241.5	208	217.5	305	262.5	203.5	262
	80%	213	225.5	226.5	284	223	226.5	328	291	207.5	291.5
	90%	219	235.5	244	330.5	262.5	241.5	343	328	213	316
	95%	227.5	248	272	340.5	336	261	360.5	357.5	220	330
	FBP	265.5	281.5	329	364	403.5	292.5	404	409	253	357.5

Table A.1 Summary Data for FACE Gasolines

Specific Tests: FACE Gasoline:	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**
Elemental Analysis (ASTM D 5291):										
-Carbon (wt.%):										
-Lab 1	83.98	84.41	84.97	86.47	85.47		86.71	87.92	84.15	
-Lab 4	84.00	84.44	84.19	86.45	85.47	84.96	86.69	87.03	84.14	86.24
-Average	83.99	84.43	84.58	86.46	85.47	84.96	86.70	87.48	84.14	86.24
-Hydrogen (wt.%):										
-Lab 1	16.02	15.59	15.03	13.53	14.53		13.29	12.08	15.85	
-Lab 4	16.00	15.56	15.85	13.55	14.53	15.04	13.31	12.97	15.86	13.76
-Average	16.01	15.57	15.47	13.54	14.53	15.04	13.30	12.52	15.86	13.76
Sulfur by UV Fluorescence (ppmw) (ASTM D5453)										
-CPChem COA	4	4	3	2	21	2	20	15	2	2
-Lab 4	6	4	4	2	21	2	22	15	2	2
Hydrocarbons by FIA (vol.%) (ASTM D1319):										
-Aromatics (vol.%): CPChem COA	0	4.2	2.1	29.5	12.1	5.8	33.5	35.3	0.9	27.8
-Olefins (vol.%): CPChem COA	0.4	0.7	0.4	0.4	9.9	8.6	7.8	7.9	6.2	1.0
-Saturates (vol.%): CPChem COA	99.6	95.1	97.5	70.1	78.0	85.6	58.7	56.8	92.9	71.2
Aromatics by SFC (ASTM D5186): (Lab 1):										
-MonoAromatics (wt.%)										
-Lab 1	0.7	7.8	6.0	41.4	14.2	10.0	39.3	41.2	0.4	38.7
-Lab 2		8.0		42.1	13.8		39.5	42.8		
-Average	0.7	7.9	6.0	41.75	14.0	10.0	39.4	42.0	0.4	38.7
-PolyAromatics (wt.%)										
-Lab 1	0	0	0	0.3	1.1	0	1.0	1.0	0	0.3
-Lab 2		0		0	0.9		1.2	1.5		
-Average	0	0	0	0.15	1.0	0	1.1	1.25	0	0.3
-NonAromatics (wt.%)										
-Lab 1	99.3	92.2	94.0	58.3	84.7	90.0	59.7	57.8	99.6	61.0
-Lab 2		92.0		57.9	85.0		59.3	55.7		
-Average	99.3	92.1	94.0	58.1	84.75	90.0	59.5	56.75	99.6	61.0

Table A.1 Summary Data for FACE Gasolines

Specific Tests: FACE Gasolines:	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**
Detailed Hydrocarbon Analyses by GC-FID:										
-n-paraffins (vol.%): (Targets)	**(5)**	**(5)**	**(25)**	**(25)**	**(5)**	**(5)**	**(5)**	**(25)**	**(5)**	**(25)**
-Lab 1	11.44	7.83	24.09	23.46	7.71	4.34	6.62	22.14	14.41	31.15
-Lab 2	11.87	8.15	24.76	24.73	8.03	4.46	6.85	22.83	14.37	32.12
-Average	11.65	7.99	24.43	24.10	7.87	4.40	6.73	22.49	14.39	31.64
-iso-paraffins (vol.%):										
-Lab 1	85.62	85.91	68.8	42.06	45.63	67.65	38.21	23.22	74.49	33.62
-Lab 2	86.35	85.86	70.66	42.21	46.21	67.47	38.64	22.40	74.59	33.66
-Average	85.99	86.88	69.73	42.13	45.92	67.56	38.43	22.81	74.54	33.64
-cyclo-paraffins (vol.%):										
-Lab 1	1.92	0.21	0.48	0.10	22.16	10.78	11.63	10.35	3.24	2.34
-Lab 2	1.30	0.07	0.23	0.10	19.45	11.18	11.40	10.66	3.36	2.24
-Average	1.61	0.14	0.36	0.10	20.81	10.98	11.52	10.50	3.30	2.29
-aromatics (vol.%): (Targets)	**(5)**	**(5)**	**(5)**	**(35)**	**(5)**	**(5)**	**(35)**	**(35)**	**(5)**	**(35)**
-Lab 1	0.73	6.01	4.09	34.25	11.21	8.05	34.19	35.97	1.20	32.12
-Lab 2	0.03	5.68	3.74	32.58	10.62	7.39	33.06	35.55	1.10	31.25
-Average	.38	5.84	3.92	33.41	10.92	7.72	33.63	35.76	1.15	31.69
-olefins (vol.%):										
-Lab 1	0.24	0.01	2.48	0.04	11.46	9.78	8.51	7.14	6.43	0.66
-Lab 2	0.18	0.03	0.06	0.05	13.92	9.05	7.71	6.50	6.27	0.54
-Average	0.21	0.02	1.27	.04	12.69	9.42	8.11	6.82	6.35	0.60

Appendix B

Properties of FACE Gasoline Blends with Ethanol

Table B.1 Summary Data for FACE Gasoline Blends with Ethanol

Specific Tests: FACE Gasoline Blend:	**A**				**B**			
Ethanol Content: (Vol. %)	**0**	**10**	**15**	**30**	**0**	**10**	**15**	**30**
Ethanol Content (Vol. %) (ASTM D5599)	0	10.12	14.69	29.90	0	9.95	14.73	30.16
Research Octane Number (RON) (ASTM D2699):								
-Lab 1	84.3	92.2	95.1	103.2	95.8	101.5	103.9	106.7
-Lab 2	83.9	92.3	95.1	101.7	96.0	100.8	102.3	105.0
-Lab 3	83.5	91.7	94.6	102.5	95.7	101.2	103.1	106.9
-Lab 4		91.6	94.5	101.8		100.9	102.6	105.3
-Average	83.9	92.0	94.8	102.3	95.8	101.1	103.0	106.0
Motor Octane Number (MON) (ASTM D2700):								
-Lab 1	83.6	87.8	89.0	91.2	92.3	93.6	93.6	93.4
-Lab 2	83.3	87.4	89.1	91.7	93.1	93.5	93.4	93.1
-Lab 3	83.5	88.1	89.3	91.1	91.9	93.3	93.4	93.3
-Lab 4		88.4	90.1	91.6		93.5	93.6	93.3
-Average	83.5	87.9	89.4	91.4	92.4	93.5	93.5	93.3
Sensitivity (RON-MON)								
-Lab 1	0.7	4.4	6.1	12.0	3.5	7.9	10.3	13.3
-Lab 2	0.6	4.9	6.0	10.0	2.9	7.3	8.9	11.9
-Lab 3	0	3.6	5.3	11.4	3.8	7.9	9.7	13.6
-Lab 4		3.2	4.4	10.2		7.4	9.1	12.0
-Average	0.4	4.1	5.4	10.9	3.4	7.6	9.5	12.7
API Gravity (API°) (ASTM D4052):								
-Lab 1	74.9	71.64	70.66	66.1	71.31	69.0	67.72	63.75
-Lab 4		71.6	70.6	66.0		69.0	67.6	63.8
-Average	74.9	71.62	70.63	66.05	71.31	69.0	67.66	63.77
Density (ASTM D4052):								
-Lab 1	0.6849	0.6959	0.6992	0.7154	0.697	0.7050	0.7096	0.7240
-Lab 4		0.6966	0.6999	0.7161		0.7055	0.7106	0.7244
-Average	0.6849	0.6963	0.6996	0.7158	0.697	0.7053	0.7101	0.7242
RVP (psi) (D5191): Lab 1	8.3	9.5	9.4	9.1	7.3	8.7	8.6	8.3
Net Heat of Combustion (BTU/lb) (ASTM D4809):		18308						
Net Heat of Combustion (BTU/lb) (ASTM D240):								
-Lab 1	19266	18294	18080	16751	19207	18319	17941	16631
-Lab 4	19236	18208	17963	16487	19168	18307	17696	16234
-Average	19251	18251	18021	16619	19187	18313	17818	16432

Table B.1 Summary Data for FACE Gasoline Blends with Ethanol

Specific Tests: FACE Gasoline Blend:	**C**				**H**			
Target Ethanol Content: (Vol. %)	**0**	**10**	**15**	**30**	**0**	**10**	**15**	**30**
Ethanol Content (Vol.%) (ASTM D5599)	0	10.18	14.62	29.49	0	10.16	14.59	30.34
Research Octane Number (RON) (ASTM D2699):								
-Lab 1	85.0	91.8	95.1	101.2	87.0	91.9	94.1	99.3
-Lab 2	84.0	92.0	95.0	101.4	86.9	92.7	94.1	99.6
-Lab 3	84.0	91.7	94.6	101.9	86.9	92.0	93.7	99.5
-Lab 4		91.4	94.5	101.5		91.6	94.6	99.1
-Average	84.3	91.7	94.8	101.5	86.9	92.1	94.1	99.4
Motor Octane Number (MON) (ASTM D2700):								
-Lab 1	83.0	87.6	89.3	92.1	79.7	82.1	83.5	86.1
-Lab 2	83.0	86.8	88.0	92.4	79.3	82.0	83.1	88.5
-Lab 3	82.9	87.6	88.7	90.9	79.9	81.7	82.9	85.8
-Lab 4		88.1	89.0	91.4		82.8	83.9	87.7
-Average	83.0	87.5	88.8	91.6	79.6	82.2	83.3	87.0
Sensitivity (RON-MON)								
-Lab 1	2.0	4.2	5.8	9.1	7.3	9.8	10.6	13.2
-Lab 2	1.0	5.2	7.0	9.0	7.6	10.7	11.0	11.1
-Lab 3	1.1	4.1	5.9	11.0	7.0	10.3	10.8	13.7
-Lab 4		3.3	5.5	10.1		8.8	10.7	11.4
-(RON)avg – (MON)avg	1.3	4.2	6.0	9.9	7.3	9.9	10.8	12.4
API Gravity (API˚) (ASTM D4052):								
-Lab 1	73.2	70.69	69.43	65.23	54.81	54.16	53.75	52.47
-Lab 4		70.7	69.3	65.2		54.4	53.8	52.7
-Average	73.2	70.7	69.4	65.2	54.8	54.3	53.77	52.6
Density (ASTM D4052):								
-Lab 1	0.6906	0.6991	0.7035	0.7186	0.7587	0.7614	0.7631	0.7684
-Lab 4		0.6997	0.7043	0.7192		0.7610	0.7636	0.7678
-Average		0.6994	0.7039	0.7189	0.7587	0.7612	0.7633	0.7681
RVP (psi) (D5191): Lab 1	7.5	8.6	8.5	8.3	7.6	8.8	8.7	8.4
Net Heat of Combustion (BTU/lb) (ASTM D4809):	19186	18198	17955	16692				16265
Net Heat of Combustion (BTU/lb) (ASTM D240):								
-Lab 1	19257	18375	18012	16739	18675	17891	17550	16369
-Lab 4					18576	17809	17408	16322
-Average	19257	18375	18012	16739	18625	17850	17479	16345

Table B.1 Summary Data for FACE Gasoline Blends with Ethanol

Specific Tests: FACE Gasoline Blend:	A				B			
Target Ethanol Content	**0**	**10**	**15**	**30**	**0**	**10**	**15**	**30**
Ethanol Content (Vol.%):								
-ASTM D5599	0	10.12	14.69	29.90	0	9.95	14.73	30.16
-Detailed Hydrocarbon Analysis - GCFID								
-Lab 1	0	10.00	14.63	30.17	0	10.01	14.76	30.14
Elemental Analysis (ASTM D 5291):								
-Carbon (wt.%):								
-Lab 1	84.43	81.78	79.41	73.06	84.65	81.72	80.29	73.46
-Lab 4	84.33	80.85	78.23	73.61	84.71	81.10	79.21	73.80
-Average	84.38	81.31	78.82	73.33	84.68	81.41	79.75	73.63
-Hydrogen (wt.%):								
-Lab 1	15.43	15.27	14.84	14.46	14.73	14.62	14.42	13.87
-Lab 4	16.06	15.73	15.48	15.15	15.61	15.40	15.25	14.87
-Average	15.75	15.50	15.16	14.81	15.17	15.01	14.83	14.37
-Oxygen (wt.%) (ASTM D5599) Lab 4:	0	4.00	5.78	11.50	0	3.89	5.71	11.47

Specific Tests: FACE Gasoline Blend:	C				H			
Target Ethanol Content	**0**	**10**	**15**	**30**	**0**	**10**	**15**	**30**
Ethanol Content (Vol.%):								
-ASTM D5599	0	10.18	14.62	29.49	0	10.16	14.59	30.34
-Detailed Hydrocarbon Analysis - GCFID								
-Lab 1	0	10.27	14.83	29.88	0	10.21	14.68	30.40
Elemental Analysis (ASTM D 5291):								
-Carbon (wt.%):								
-Lab 1	84.47	82.00	79.98	73.36	87.68	84.02	84.01	76.24
-Lab 4	84.19	80.77	79.09	73.53	87.20	83.16	81.50	76.26
-Average	84.33	81.38	79.54	73.45	87.44	83.59	82.76	76.25
-Hydrogen (wt.%):								
-Lab 1	14.94	14.65	14.65	14.05	12.05	11.99	12.07	12.18
-Lab 4	15.85	16.68	15.23	15.09	13.00	13.05	12.92	13.16
-Average	15.40	15.67	14.94	14.57	12.53	12.52	12.50	12.67
-Oxygen (wt.%) (ASTM D5599) Lab 4:	0	4.01	5.72	11.29	0	3.68	5.27	10.88

Table B.1 Summary Data for FACE Gasoline Blends with Ethanol

Specific Tests: FACE Gasoline Blend:	A				B			
Target Ethanol Content	**0**	**10**	**15**	**30**	**0**	**10**	**15**	**30**
Distillation (˚F) (ASTM D86) Lab 1:								
IBP	90	106	99	99	97	105	103	101
5%	122	127	122	126	133	128	126	129
10%	140	134	131	135	149	135	134	138
20%	165	145	144	146	175	147	146	149
30%	186	153	152	153	196	155	154	155
40%	198	159	156	156	209	165	159	159
50%	204	202	159	158	214	211	165	161
60%	207	208	204	159	218	217	214	162
70%	210	211	210	160	221	219	219	163
80%	213	214	213	161	226	225	224	165
90%	219	222	219	211	236	234	234	230
95%	228	233	229	224	248	247	246	242
FBP	262	261	263	260	280	271	270	266

Specific Tests: FACE Gasoline Blend:	C				H			
Target Ethanol Content	**0**	**10**	**15**	**30**	**0**	**10**	**15**	**30**
Distillation (˚F) (ASTM D86) Lab 1:								
IBP	93	104	102	107	98	96	105	106
5%	126	126	123	130	127	123	125	127
10%	139	131	131	136	143	132	134	138
20%	157	140	140	145	170	145	147	152
30%	174	147	147	151	194	153	156	159
40%	188	153	153	156	213	167	161	163
50%	201	183	157	159	229	217	182	166
60%	210	208	176	161	243	236	235	169
70%	218	217	215	162	263	255	253	175
80%	227	226	223	165	291	283	282	268
90%	245	244	241	233	329	322	323	312
95%	274	274	269	261	357	351	351	343
FBP	330	331	322	324	408	401	407	396