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Strategies and Issues in Correlating Diesel Fuel Properties with Emissions

Staff Discussion Document

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Assessment and Standards Division
Office of Transportation and Air Quality
U.S. Environmental Protection Agency

NOTICE

This technical report does not necessarily represent final EPA decisions or positions.
It is intended to present technical analysis of issues using data that are currently available.
The purpose in the release of such reports is to facilitate the exchange of
technical information and to inform the public of technical developments which
may form the basis for a final EPA decision, position, or regulatory action.

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Section I Introduction

This staff discussion document describes technical issues related to an assessment of the effect of changes in diesel fuel parameters on the emissions of hydrocarbons (HC), particulate matter (PM) and oxides of nitrogen (NOx). It is intended as a starting place for discussion and comment. It is not a final technical report.

A. Regulatory Context

1. Federal and State Regulation of Diesel Fuel Parameters

EPA's desire to quantify the emission effects of diesel fuel parameter changes stems from growing state interest in reducing criteria pollutant emissions by regulating diesel fuel properties. Federal law and regulations control sulfur and aromatic content and the cetane index of highway diesel fuel introduced into commerce as of October 1, 1993.[1] Except for California,[2] no state had regulated similar aspects of diesel fuel until April 2000, when Texas adopted its Low Emission Diesel (LED) rule for the Dallas metropolitan area,[3] and later amended the same rule to expand the geographic scope of the covered area and to further restrict sulfur levels.[4] Like the California rule (implemented in October, 1993) the Texas rule (to be implemented in April, 2005[a]) controls sulfur and aromatic hydrocarbon content of diesel fuel for both highway and nonroad engines; Texas also controls the cetane number of diesel fuel.[b]

The Ozone Transport Commission (OTC) also in 2000 began considering a model rule that could be adopted by its member states wanting to regulate the content of diesel fuel.[c] The OTC model rule would have required a high cetane number in diesel fuel for both highway and nonroad engines. The OTC states were interested in potential emission reductions of both NOx and HC.

We also are aware of additional states that have considered or are considering controls of diesel fuel parameters. While there are a number of issues related to state fuel regulations, including fuel supply, actual use of the required fuel, and cost, one important unanswered question has been the amount of emission benefits in vehicles using the alternate fuel. As a result of the substantial

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[a] Although the rule as currently adopted requires implementation by May, 2002, Texas has proposed revising the rule to delay implementation until April, 2005, and has requested that EPA "parallel process" this proposed revision. See text of revisions to 30 Tex. Admin. Code, Chapter 114, Section 114.319, proposed by TNRCC on May 10, 2001, at the following website: http://www.tnrcc.state.tx.us/oprd/sips/houston.html. This proposed revision implements legislation adopted by the Texas Legislature (HB 2912) prohibiting implementation of this low emission diesel rule until February, 2005.

[b] Although California does not set a regulatory standard for cetane number, it does require use of a reference fuel with a specific cetane number (identical to the Texas regulatory standard) in determining whether alternative formulations (which do not meet the 10% aromatics content standard) have equivalent emissions reductions. Alternative fuel formulations with equivalent emissions reductions can meet the California diesel fuel requirements.

[c] To date, OTC has not adopted a model rule for diesel fuel control, and is no longer actively considering it.

recent interest in diesel fuel control and the lack of comprehensive information on the benefits of such fuel, in November 2000, EPA initiated an effort to evaluate the emission benefits of varying diesel fuel parameters.

2. The Texas Low Emission Diesel Rule

In particular, EPA must respond to the Texas proposed State Implementation Plan (SIP) revisions seeking emissions reduction credit for its LED rule. Texas submitted to EPA its LED rule as one of many control measures to be included in its SIP for meeting the National Ambient Air Quality Standards for ozone in the Dallas and Houston areas. Because we must complete rulemaking action on the proposed Houston SIP revisions by October 15, 2001, in order to meet a court-ordered deadline, we needed to know as soon as possible whether our analysis supported approval of the NOx reductions claimed for the LED SIP revision. The analysis described in this staff discussion document was designed to help us answer this question, as well as help provide a consistent response to future questions on the emission benefits of diesel fuel controls.

In its proposed SIP revisions, Texas claims the LED rule will provide significant reductions in emissions of oxides of nitrogen (NOx). In developing the NOx emission reduction estimates, Texas assumed its LED fuel would be similar to California diesel fuel. For highway engines with electronic controls (i.e., 1990 and later models for the most part), Texas estimated NOx reductions at 5.7%, based on regression equations in the Heavy Duty Engine Working Group (HDEWG) report, a project of the Coordinating Research Council (CRC). For pre-1990 highway engines and for all non-road diesel engines, Texas estimated NOx reductions at 7%, based on California Air Resources Board (CARB) test data from 1988.[5]

Given the absence of a publicly reviewed emissions model for diesel fuel parameters, we were concerned about the accuracy, magnitude, and consistency of estimates of the emission reduction benefits of increasing cetane and limiting aromatics in diesel fuel used in the current fleet. Many studies of the emissions effects of diesel fuel parameters have been done in the past several years that were not included in the Texas analysis.

In particular, the HDEWG report, which is included in our list of data sources (Appendix A,) examined, among other things, the effects of cetane number and aromatic content on emissions from 1998 and 2004 prototype heavy duty diesel engines. The 5.7% estimate being used by Texas is drawn from the testing done on an engine meeting the 1998 standards and presumes that all technologies and model years from 1990 forward will respond similarly to changes in fuel properties.

Also, for the older highway engines (i.e., pre-1990 model years), and for the entire nonroad diesel engine fleet, Texas relied on CARB "test data from 1988" as support for its estimate of 7% NOx reductions. CARB's Staff Report and Technical Support Document for its proposed diesel fuel regulation (both dated October 1988) indicate the source of this data is CARB's analysis of the preliminary results of the CRC test program for the Phase 1 VE-1 project.[6] As of the time of the

1988 CARB Report, testing in the VE-1 project had been completed for two engines, a Cummins NTCC 400 engine and a Detroit Diesel DDAD 60 engine. After CARB's final determination of the benefits of its diesel fuel control program in 1988, the Phase 1 VE-1 project was completed, including testing on a third engine, and the report was published in 1989. CRC went on to complete a Phase 2 to the VE-1 test program, and eventually a VE-10 test program. Numerous other studies have also been completed since the 1988 CARB Report.

While the engines tested in the Phase 1 VE-1 study represent some pre-1990 technologies, additional test data is available on this portion of the fleet. In addition, it is not necessarily appropriate to use the Phase 1 VE-1 results alone to estimate NOx reductions in all nonroad diesel engines. We believe that a more thorough review of the existing data, including studies completed since 1988, is an important element of estimating the benefits of diesel fuel controls on the in-use fleet.

B. Objectives and Scope of Research

The primary goal of this EPA project is to provide an objective estimate of the effect of changes in diesel fuel parameters on emissions of NOx, HC and PM. As such, our objective is to provide equations for calculating fuel-based emissions changes of these pollutants for various commonly-used diesel engine technologies.

This research project has been subject to tight time constraints, due to the need to meet the deadlines for EPA rulemaking on the Houston SIP. For this reason, we have not done any vehicle testing; instead we developed a regression model from existing test data.

Our study has focused on the fuel parameters, vehicles, and pollutants that are currently of greatest concern in State Implementation Plans (SIPs). Thus, the study was primarily concerned with the NOx, HC and PM benefits of cetane and aromatics on emissions from engines commonly used in heavy-duty highway trucks. However, many of the studies included information on CO, HC and BSFC, so we also collected data on these parameters and may develop regression equations for them in the future. Data on toxic emissions was quite limited, so our analysis of these emissions was qualitative. Similarly, there were few data available on the effects of diesel fuel parameters in light duty vehicles. Since light duty diesel vehicles comprise a very small fraction of the current fleet, we conducted only a literature survey of the relevant light duty emissions studies. And, while the effects of diesel fuel changes on nonroad equipment such as construction and farming equipment are of considerable interest due to their contribution to in-use emission inventories, lack of data made it necessary for us to extrapolate our findings from highway vehicles to nonroad equipment.

Where data was available, we used a regression model approach to analyze our results and to develop a quantitative relationship between fuel parameters and emissions changes. We considered the benefits of both a traditional regression approach and a principal component analysis approach that uses eigenvectors to eliminate colinearity between independent variables.[7]

C. Interaction with Stakeholders

To assure that our analysis benefitted from data and expertise outside the EPA, we have made a deliberate effort to work with external stakeholders from the beginning of our work on this topic. In order to inform stakeholders of the work that EPA would be doing to look at the effects of diesel fuels on emissions, a presentation was made to the Federal Advisory Committee Act's Mobile Sources Technical Review Sub-committee and informational letters were sent to stakeholders. The first letter was a general notice to stakeholders, the second was a request for any pertinent data that could be included in our study. We established an e-mail list for individuals known to have an interest in our work, with periodic messages sent to inform members of the status of our work. We also developed a web site (http://www.epa.gov/otaq/models/analysis.htm) to share our plans and intermediate work products.

In addition to general interaction with stakeholders, we have also worked particularly closely with the California Air Resources Board (CARB) and the Department of Energy (DOE). CARB staff has significant interest and experience in fuel emissions modeling (e.g. their Predictive Model for gasoline vehicle emissions). DOE staff and their consultants also have interest and expertise in this area and have an independent project to develop a principal component analysis for quantifying the relationship between fuel parameters and emissions.

D. Request for Comments

While more time and additional research could improve our analysis, within the time limits of the Houston SIP rulemaking, we performed a comprehensive review and analysis of all pertinent, available data, and produced what we believe is a reasonable model of the percent reductions of the relevant emissions as a function of fuel parameter changes.

However, in this process, a number of issues have been raised , both regarding the details of the regression analysis and regarding its possible application. To assure that our model represents the best current scientific understanding of these emission effects, we are planning a workshop in August 2001 to discuss technical issues relating to our analysis of the emission effects of varying diesel fuel parameters. For information on this workshop, please see our website (http://www.epa.gov/otaq/models/analysis.htm). Comments on this staff discussion document and our analysis may also be sent to EPA in writing prior to the workshop date. Written comments can be submitted to Tia Sutton at sutton.tia@epa.gov, or through regular mail to:

Tia Sutton
U.S. EPA National Vehicle and Fuel Emissions Laboratory
2000 Traverwood Drive
Ann Arbor, MI 48105

At the conclusion of the workshop, EPA will consider the comments received and will revise our analysis in response to comments. We then plan to publish a technical report that summarizes our work and conclusions.

Section II What Data Was Used?

We began the process of assembling data for use in developing a fuel property/emissions model by conducting literature searches, reviewing lists of relevant data sources that had been assembled by other researchers for use in similar analyses, and making requests from stakeholders for data that may not have been public. Given the short timeframe permitted for developing a model, we set a deadline of February 15, 2001 for receiving data from stakeholders. We received no additional data from stakeholders.

Regarding lists of data sources from other researchers, we reviewed the bibliographies of Sierra Research's Maricopa County study[8] and the Oak Ridge National Laboratory's eigenvector model report[9]. We also reviewed lists of suggested data sources provided by DaimlerChrysler and the Georgia Department of Natural Resources. Once we had assembled a complete list of prospective data sources, we reviewed each study to verify that it contained the actual raw data that the report or study described. If the raw data was not provided, we made attempts to contact the authors. Only one such attempt was successful, for SAE paper number 922214, and so this study was included in our analysis. The remaining papers without raw data which are excluded from this analysis are listed in Appendix A.

We reviewed the studies to verify that they met certain criteria consistent with the goals of the project. These criteria are described in Section II.A below. As a result of this review, only 35 of the full set of 70 studies were retained for our analysis. We then entered the data into a database specifically designed for this project, making adjustments to ensure consistency in units, corrections for emissions drift over time, and balancing of repeat measurements. The engines were then each assigned to a technology group designed specifically for this project as described in Section II.C below. Finally, the different test cycles used to collect emissions data were assessed to determine how well they represented the Federal Test Procedure (FTP), which is the current best representation of the operation of in-use heavy-duty highway engines among the available test data. All of these steps are described in the remaining portions of this Section. Additional details can be found in the final report from Southwest Research Institute[10].

A. Criteria for choosing data sources

As described in Section I, the model we have developed is intended to represent conventional diesel fuel effects on emission from heavy-duty highway compression-ignition engines[d]. The data that we considered for use in the development of the model was screened to ensure that it met certain criteria consistent with this goal.

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[d] Although essentially all available data was collected on highway engines, the models can also be applied to the nonroad fleet as described in Section IV.E.

To begin with, we limited our analysis to No. 1 and No. 2 diesel fuel and related blends that can be used in a typical heavy-duty diesel engine without engine modifications. As a result we excluded all emulsions and oxygenated blends with more than 20 vol% oxygenate. We also excluded fuels that were made entirely from pure chemicals rather than refinery streams. We did not specifically exclude Fischer-Tropsch fuels, nor did we limited ourselves to diesel fuels containing less than 500 ppm sulfur. However, some fuels were excluded as being not representative of current or potential future in-use fuels as described in more detail in Section B.3 below.

We also limited this study to engines that had already been sold commercially or had a high probability of being sold in the future. Engines with experimental technologies that had no immediate plans for commercialization, such as those with innovative combustion chamber geometries, were excluded. Likewise, single-cylinder research engines were also excluded from consideration even though the associated full-size parent engine might have been appropriately included in the database had it been tested. Single-cylinder engines do not appear in heavy-duty applications. By definition they have lower total horsepower and displacement, both of which are parameters in our technology group definitions as described in more detail in Section II.C below. Unless we were to make the assumption that single cylinder engines respond in the same way as their parent engine to changes in fuel properties, we would have to define new technology groups specific to single-cylinder engines. Light-duty engine and vehicle data was separated for an independent analysis (see Section VI). Nonroad engines were not specifically excluded from the analysis, but the paucity of nonroad engine data made it necessary for us to evaluate nonroad engine fuel effects separately, as described in Section IV.E.

The type of testing also played a role in determining if a given study should be included in our analysis. For instance, since we were primarily interested in fuel effects on emissions, we excluded all studies that did not test at least two different fuels on the same engine. Chassis tests were not specifically excluded from the database, but since the vast majority of heavy-duty testing is done on engines instead of chassis, the inconsequential amount of chassis test data was not included in our model development process.

The complete list of data sources that we considered for our analysis is given in Appendix A. Studies that were excluded from our analysis are separated and categorized according to the reason for their exclusion.

B. Preparation of database

1. Database structure

In designing the structure of the database and the fields that would be included, it was our intention to include all information that had any potential for helping us to quantify the relationship between diesel fuel properties and emissions. In addition, we also wanted to ensure that a wide variety of issues could be investigated once the database was assembled, including issues which were not immediately germane to our primary goal of correlating diesel fuel properties with emissions. This secondary goal is of broad and continuing interest to the EPA as we continue our efforts to understand and control pollution from diesel-powered engines and vehicles. Towards these ends, we selected a wide variety of fuel, engine, and test parameters to include in the database.

The database was divided into three separate files:

fbat_ad	File containing a complete description of every fuel, including compositional, chemical, and combustion characteristics.
equip_ad	File containing a complete description of every engine, include both engine design characteristics and elements that may have been changed subsequent to production, such as aftertreatment and EGR
etest_ad	File containing individual test descriptions and emission results

Data source IDs were used to link specific fuels, engines, and emission estimates across the three files. We also designed a fourth file in which modal data could be recorded. However, since so few studies included the raw modal data and we did not have sufficient time to investigate modal effects, no data was entered into this fourth file. A complete description of the fields for all three database files is given in Appendix B.

2. Entering data

The primary concern as data was being entered into the database was consistency of units. For the most part these conversions were straightforward, and are described in more detail in the SwRI final report[10]. In some cases, however, the fuel property unit conversions were not straightforward due to ambiguity in either a given study or the database structure itself. In these cases decisions were made that were intended to maximize the useful amount of data. These decisions are summarized below:

Viscosity - The viscosity of a fuel can be measured at different temperatures. In cases where more than one temperature was used, the measurement closest to 40 °C was entered into the database. If only one viscosity measurement was made, it was entered into the database without regard to test temperature.

Biodiesel - Biodiesel blends were grouped with all other oxygenates, with its corresponding wt% oxygen level being entered into the database. An attempt was made to determine if the oxygenate type had an effect on emissions that was separate from the oxygen effect. This assessment is discussed in more detail in Section IV.D.

Oxygen - If an oxygenate was not added to a fuel and the oxygen level was not measured, it was assumed to be zero. If oxygen was measured, we used the measured value even if doing so included the contribution of, for instance, cetane improver additives to the oxygen content of the fuel.

Properties of cetane-enhanced fuels - If the properties of a fuel were measured before a cetane improver was added to the fuel but not afterward, the properties of the base fuel were considered to be applicable to the additized fuel as well, with the exception of cetane number.

Concentration of cetane improver additives - Our database required that the concentration of cetane improver additives be entered as vol%. If a study provided the concentrations in terms of wt%, the conversions were made using the following equation:

$$\text{vol\%} = \text{wt\%} \text{ X fuel specific gravity} / b$$

where b is the specific gravity of the cetane improver additive[e].

Cetane increase due to additives - If the increase in cetane number which resulted from the addition of a cetane improver additive was not given in the study, it was estimated from a correlation given in SAE paper number 972901. This correlations is:

$$CNI = a \times CN^{0.36} \times G^{0.57} \times C^{0.032} \times \ln(1 + 17.5 \times C)$$

Where:

CNI = Predicted cetane number increase due to an additive
a = 0.16 for 2-ethylhexylnitrate and 0.119 for di-tertiary butylperoxide
CN = Base cetane number
G = Fuel API gravity
C = concentration of additive in vol%

Cetane index - If the cetane number of a fuel was not measured, the cetane index was used as a surrogate for cetane number. This applied to all fuels in two studies, for a total of thirteen test fuels (out of 300 in the database).

Aromatics test methods - The database required total aromatics to be entered in units of vol% as established from an FIA test method (ASTM D 1319 or the equivalent). If total aromatics was derived using supercritical fluid chromatography (SFC, from ASTM D 5186 or its

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[e] For 2-ethylhexylnitrate (EHN) this value is 0.964 according to an Ethyl data sheet on their HiTEC Cetane Improver Additive (composed of 99% 2-EHN). For di-tertiary butylperoxide (DTBP), the value of b is 0.794 according to the CRC Handbook of Chemistry and Physics.

equivalent), which produces measurements in wt%, the conversion was made using an equation derived from the California Code of Regulations, Title 13, Section 2282(c)(1):

$$\text{vol\% (by FIA)} = 0.916 \times \text{wt\% (by SFC)} + 1.33$$

If total aromatics content was not measured by an SFC test method, then alternative conversion equations were used. These conversion equations were derived specifically for this analysis and are described in Appendix C.

Total, mono, and polyaromatics - Total aromatics content is the sum of mono and polyaromatics. Thus if a study provided measurements for only two of these three properties, the third was estimated based on this relationship.

The database required mono and polyaromatics to be entered in units of wt% as established using an SFC test method. If total aromatics was not measured by an SFC test method, then the conversion to wt% by SFC was made using equations derived specifically for this analysis. These equations are described in Appendix C.

There were also situations in which aspects of the data not related to fuel properties were ambiguous. In these situations we again made decisions that were intended to maximize the usefulness of the database in the context of developing an emissions model. The primary decisions are listed below:

Hot-start versus composite FTP - If the heavy-duty transient Federal Test Procedure was used to produce composite emission measurements, these were entered into the database as UDDS cycle values. If the FTP was used to produce separate hot and cold-start emission measurements and no composite results were presented, then the hot and cold-start results were weighted at 6/7 and 1/7, respectively, to produce composite results which were then entered into the database as UDDS cycle values. If the FTP was used to produce only hot-start emission measurements, then these results were entered into the database as UDDSH cycle values. See Section II.E.2 for a more detailed discussion of test cycles.

Engine adjustments - If adjustments were made to an engine, such as changes in injection timing, addition or removal of aftertreatment, etc. these were treated as unique engines and entered into the database as such. Thus each engine value in the database refers to a set of emissions data from a single engine whose operating parameters and physical characteristics did not change during the course of testing.

Repeat measurements - There were many cases in which the same fuel was tested on the same engine multiple times. All such repeat measurements were entered into the database. Our model development approach used average repeat measurements in the term-selection stage of the analysis, and all individual repeat measurements in the coefficient estimation stage. This approach is described more fully in Section III.A.3.

Averaged emissions - If the study presented only averaged emissions resulting from multiple repeat tests of a single fuel on a single engine, the average values were entered into the database the same number of times as the number of repeat tests on which the average was based. If the number of repeat tests was unknown, it was assumed to be two.

3. Adjustments to database

Once all the data had been entered into the database and it had been reviewed for errors and inconsistencies, two different adjustments were made to ensure that the database was best suited for model development.

The first adjustment involved correcting for engine drift over time. This correction was necessary for cases in which the emissions from an engine appeared to drift upwards or downwards over the course of the study. Cases in which this drift was evident were those in which the study authors specifically looked for it by testing a single fuel - usually a reference fuel - at multiple times throughout the test program. The emissions from this fuel could then be plotted against time (usually engine hours) to determine if drift occurred. If engine drift was evident, the authors may have chosen not to correct the data itself but instead add a time parameter to the regression equations that were developed using the data in that study. This option was not available in our model because so few studies included time measurements. Thus it was necessary for us to correct the data for those studies in which engine drift was investigated and found to be significant.

Engine drift was expected to be proportional to the absolute level of emissions. In other words, the percent change in emissions for the reference fuel over time was assumed to also apply to all other emission measurements. The first step was to correlate reference fuel emissions with time to produce an equation of the following form:

$$\text{Emissions (g/bhp-hr)} = a \times t + b$$

where t is the time in engine hours and a and b are regression coefficients. This equation represents the average change in emissions for the reference fuel over time. From this equation it is evident that the emissions at time zero are equal to the constant b. The correction to the existing data is then carried out using the following equation:

$$(\text{Emissions})_{\text{measured}} \times [b/(a \times t + b)] = (\text{Emissions})_{\text{corrected}}$$

Thus if the reference fuel indicates an upward trend in emissions over time, the correction should change all emission measurements by an amount inversely proportional to this emission increase. The studies that included time-drift corrections in our database included:

- SAE 2000-01-2890
- VE-1 (Phase I)

- VE-1 (Phase II)
- VE-10

The second database adjustment involved reviewing the distribution of fuel properties to ensure that they were representative of current or expected future fuels. Although we intended to rely in part on the statistical analyses to help us identify fuels that could be considered outliers, it seemed prudent to identify those fuels in the database prior to the analysis which were significantly different than any in-use fuel or which were unlikely to arise in the future. Since such fuels lie at the edges of the fuel property ranges, they have the potential for highly influencing the regression coefficients in ways that may not be representative of the in-use diesel pool.

The distribution of fuel properties in the database was compared to distributions found in recent fuel surveys from the Alliance of Automobile Manufacturers to determine how well the database fuels represented in-use fuels. In addition, the database fuels were also compared to the Worldwide Fuels Charter proposed by manufacturers to determine whether they might be considered valid fuels in the future. Fuels that were neither representative of current fuels nor potential future fuels were identified as candidates for exclusion from the database. Particular attention was paid to heavier fuels, since the trend appears to be towards lighter fuels with lower density and higher cetane. Finally, if one of the candidate fuels appeared to be of a sort that could potentially produce rough engine operation (e.g. very low cetane), it was also highlighted for exclusion. Fischer-Tropsch fuels were not specifically excluded from the database since there are small markets where they could play a significant role. As a result, six fuels were deleted from the database, out of a total of 306. Details of the deleted fuels can be found in the final report from Southwest Research Institute[10].

C. Technology groupings

We expected that engines with different technologies would respond differently to changes in fuel properties. It therefore seemed prudent to examine ways in which the database could be subdivided to capture any technology-specific effects that might exist. Although dividing the data by model years or model year groups would be most convenient from the standpoint of correlating the results of our modeling with the in-use fleet, it became clear that engines of a given model year can have widely varying technologies, and some specific engine technologies span many model years. Thus grouping engines in our database by model years could potentially mask the true effects of changes in diesel fuel properties on emissions as effects for one type of technology were blended together with effects for another type of technology. We determined that a more precise model would result if we defined categories of engine technologies within which fuel effects on emissions would be expected to be consistent.

We began by identifying ten engine characteristics that could interact with fuels and thus produce distinct effects on emissions. These characteristics are shown in Table II.C-1.

Table II.C-1 - Engine Characteristics Used in Defining Technology Groups

Rated speed
Injector type
Aspiration
Horsepower
Displacement
Oxy catalyst
Injection control
Type of injection
Cycle
EGR

The type of injector (inline, rotary, or unit) was used as a surrogate for injection pressure. From this selection of ten engine characteristics, we produced 56 technology groups intended to represent the most likely distribution of in-use engine types. The complete list of these technology groups is given in Appendix D.

The database contained a total of 75 engines (some of which were actually duplicate engines run with different injection timings). When these engines were categorized by technology group, only 17 of the original 56 technology groups contained data. The number of engines and the percent of emission observations falling into each of these 17 technology groups are shown in Table II.C-2.

Table II.C-2
Data in each technology group

Tech Group	Number of engines	Percent of emissions data
B	4	2
F	13	18
G	2	3
H	3	1
I	1	6
L	4	4
P	3	4
Q	4	6
R	3	1
T	22	42
V	3	4
X	1	2
DD	1	1
NN	2	2
OO	3	3
ZZ	4	2

D. Test cycles

The studies that we reviewed contained data generated from many diesel engine test cycles. The following is a description of the various test cycles, both transient and steady-state, that we evaluated throughout this work and a description of the test cycles that were chosen for the model. We then describe how we selected specific test cycles for inclusion in our model. In doing so, we aimed at selecting those cycles that were most representative of in-use operations.

1. Transient Cycles

The only transient test cycle used in the fuel studies being considered for inclusion in our database is the EPA transient test cycle that is used to certify on-highway heavy-duty diesel engines in the U.S. Because nearly all of the engines tested in these studies were on-highway engines and transient conditions can significantly affect particulate emissions, this is the preferred test cycle for inclusion in our model.

The EPA transient test cycle is commonly referred to as the Federal Test Procedure (FTP)[f], as it is the test cycle used for official emissions testing of diesel engines in the US.
The heavy-duty, on-highway FTP consists of four phases and a variety of different speeds and loads that are sequenced to simulate the urban operation running of the vehicle that corresponds to the engine being tested. The average load factor of the heavy-duty FTP cycle is roughly 20 to 25 percent of the maximum engine horsepower available at a given speed. The cycle weighting factors signify medium to high exhaust gas temperatures. In our database, we refer to the EPA transient test as the UDDS (urban dynamometer driving schedule). The EPA transient cycle run with a hot start only is referred to as UDDSH.[g]

2. Steady-State Cycles

The U.S. 13-mode duty cycle, as defined in 40 CFR § 336, consists of 13 sequential steady-state operating regimes with defined minimum sampling times of 4.5 minutes and maximum sampling times of 6 minutes. The speed for each mode must be held within +/- 50 rpm for each mode and the load for each mode must be within +/- 2% of the maximum available torque for each mode. The test cycle consists of three idle sample points, as well as intermediate speed, and rated speed sample modes. The intermediate speed is typically defined as a peak torque speed. The rated speed is defined as a maximum measured, full power speed. The loads correspond to: 2%, 25%, 50%, 75%, and 100% of maximum available torque at a given test speed.

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[f] *CFR Title 40, Part 86.1333.*

[g] *EPA's Mobile Source Observation Database (MSOD), the database of in-use vehicle test result data, uses UDDS as a test procedure value. However, this may also tend to be referred to by others as an FTP test cycle. Our model did draw from MSOD on the data design, with a key distinction being that MSOD distinguishes between test procedures and schedules while this model does not.*

The ECE R49 cycle (also called the EEC 88/77 cycle) is the 13-mode steady-state test cycle for heavy-duty diesel engines which was used for certification of heavy-duty engines in Europe until October 2000. The test cycle is similar to the US 13-mode cycle, as both cycles have identical running conditions. However, the R49 has different weighting factors at the idle speeds and is characterized by high engine loads.

The Japanese 13-Mode test cycle is a steady state test cycle that replaces the Japanese 6-mode cycle for testing heavy-duty engines. This test cycle places importance on low speed/ low power conditions, made evident by the fact that the cycle weight percentages are relatively low at high power. For example, for modes with loads of 80-95 percent, the weights vary from 0.037 to 0.055. In contrast, for the European and US 13-mode tests, the weights at high power (loads of 75-100%) are considerably higher, 0.08 and 0.08 to 0.25, respectively.

The AVL 8-mode is a steady-state engine test procedure for heavy-duty diesel engines consisting of eight sequential engine operating points. The cycle was developed to simulate the FTP transient cycle for heavy-duty engines for pollutants other than PM, so the exhaust emission results are closely correlated for the two test cycles for HC and NOx.

The ISO 8178 procedure is a collection of various steady state test cycles for non-road applications; with type C1 being an 8-mode, nonroad heavy-duty diesel cycle. While this is a steady-state test cycle, it is commonly referred to as the nonroad FTP cycle.

3. Choice of Test Cycles

In selecting data to include in our models, the choice of test cycle was considered to be very important. Data generated from UDDS transient cycle was preferred, as this cycle most closely represents in-use conditions. When a specific study tested an engine-fuel combination using the EPA transient test, that data was used to developed our models and data for that engine-fuel combination using all other test cycles was excluded. Transient cycle data represents the majority of the data in the database, 1195 observations. A number of studies only measured hot-start transient emissions. When this was the case, we included this data in our database and considered this data to be satisfactory when developing our models and preferred over steady-state data, if the latter were also available. As hot-start results comprise 6/7 of the composite value, we concluded that fuel effects measured using the hot-start transient test could be considered representative of composite results.

The use of steady-state data was considered in the development of the HC and NOx emission models when transient data was not available. In the case of PM emissions, only transient test data was used to develop the relationships between fuel properties and emissions. Steady-state data was not used to develop the PM models due to the importance of transients in particulate formation in diesel engines.

With respect to HC and NOx emission data, we included data from a steady-state cycle if the cycle contained a wide variety of operating modes, including those at high loads, and the weighting factors for the high load mode were similar to those of the EPA 13-mode cycle or the ECE R49 cycle. This led us to include data from the R49 and the AVL 8-mode steady-state test cycles into the final model. Practically, as most of the studies which utilized one or more of the steady-state cycles listed in the database also utilized the UDDS, much of the steady-state data was not included in the development of the NOx and HC models. In all, 74 observations were excluded from the model due to test cycle.

Our decision to include certain steady-state NOx and HC emission data in the model is confirmed by a previous study that found that fuel modifications produce similar changes in emissions over the R49 and the heavy-duty FTP tests.[h] This study concluded that the effects of fuel property changes on emissions were similar and that general extrapolations of effects from one data set to another are reasonable.

E. Summary statistics of data

This Section provides information on the data in our database, including distribution of fuel properties, test cycles, and model years. This information can be used to assess the degree to which the data used to develop our model is representative of in-use fuels and engines. For instance, we have made use of the distribution of fuel properties to determine the valid range limits of our model (see Section III.C.3). The summaries in this Section include all data in the database, i.e. no outliers identified during the analysis or observations with incomplete data have been excluded in these summaries, unless specified otherwise.

1. Fuel properties

We plotted the distribution of a selection of fuel properties for fuels in our database against the same distribution for AAM surveys. In general, the database included a wider range of fuel properties than the surveys with a tendency towards cleaner fuels (i.e. lower aromatics, lower density, higher cetane). This result is advantageous for our model because the model will most often be used to predict the benefits of cleaner-than-average fuels.

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[h] *R. Lee, J. Pedley, C. Hobbs, "Fuel Quality Impact on Heavy Duty Diesel Emissions: -A Literature Review", SAE 982649.*

Figure II.E.1-1
Distribution of aromatics

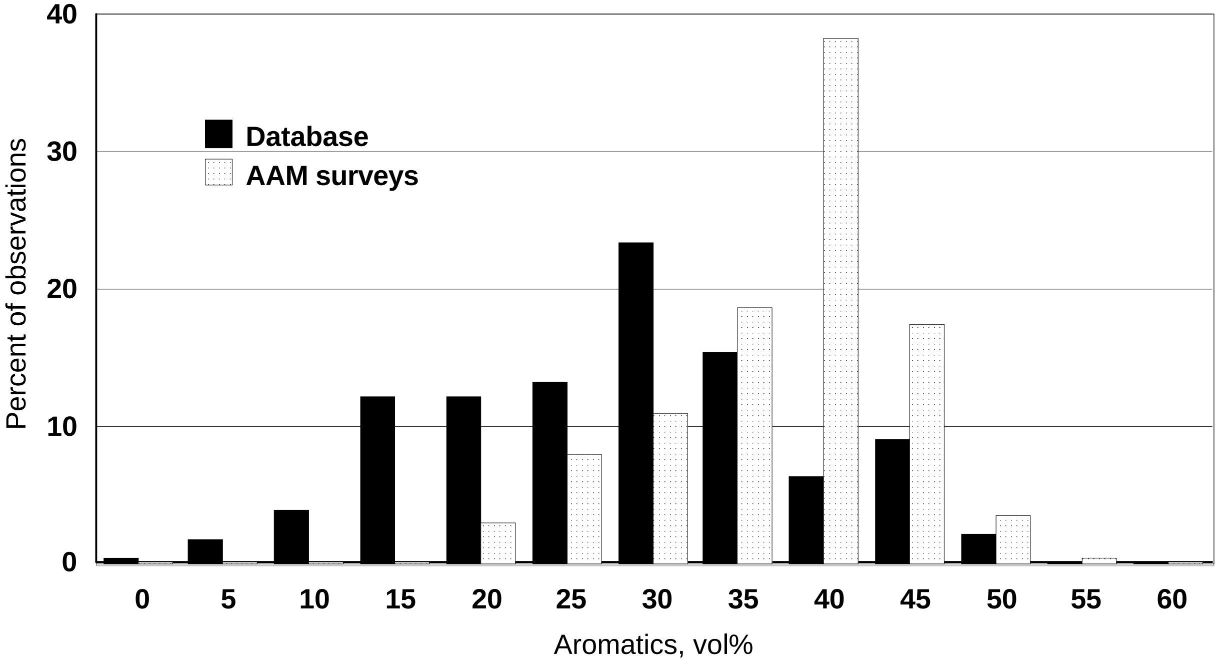


Figure II.E.1-2
Distribution of total cetane number

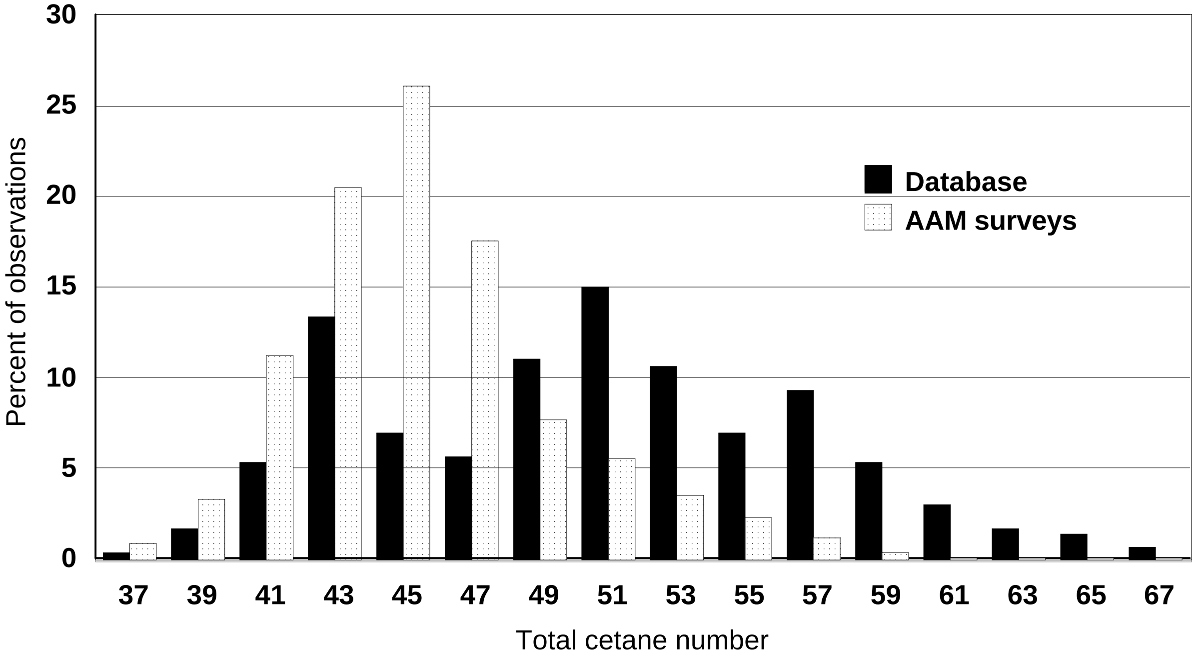


Figure II.E.1-3
Distribution of specific gravity

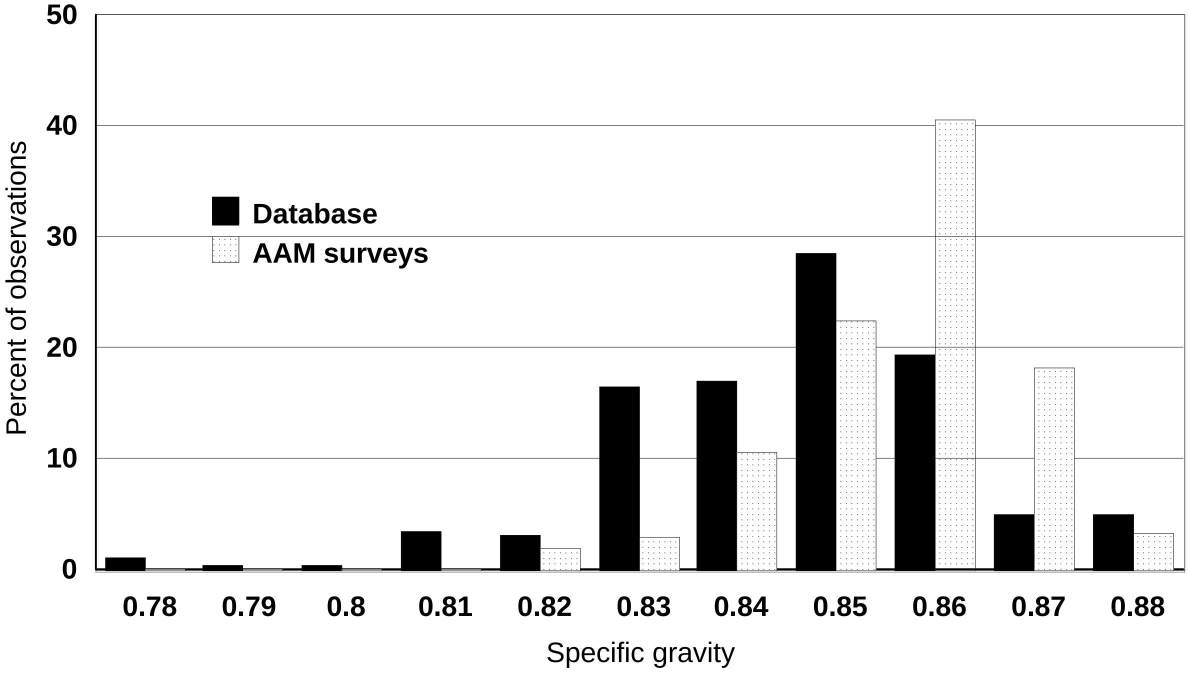


Figure II.E.1-4
Distribution of T50

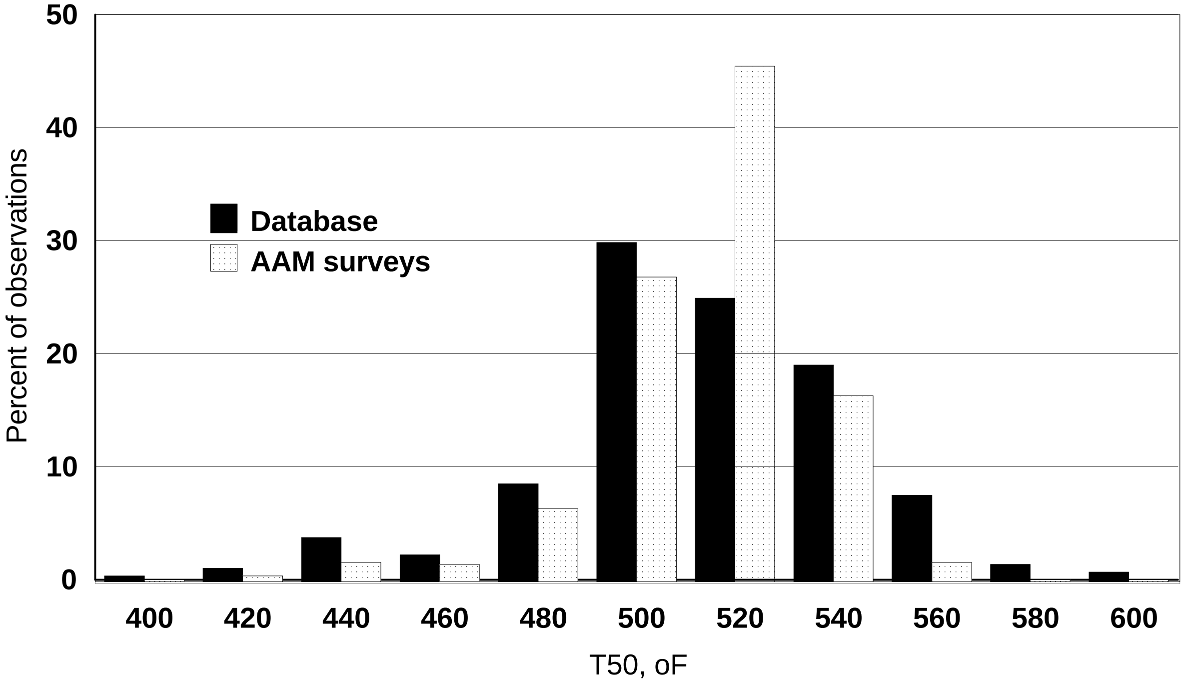
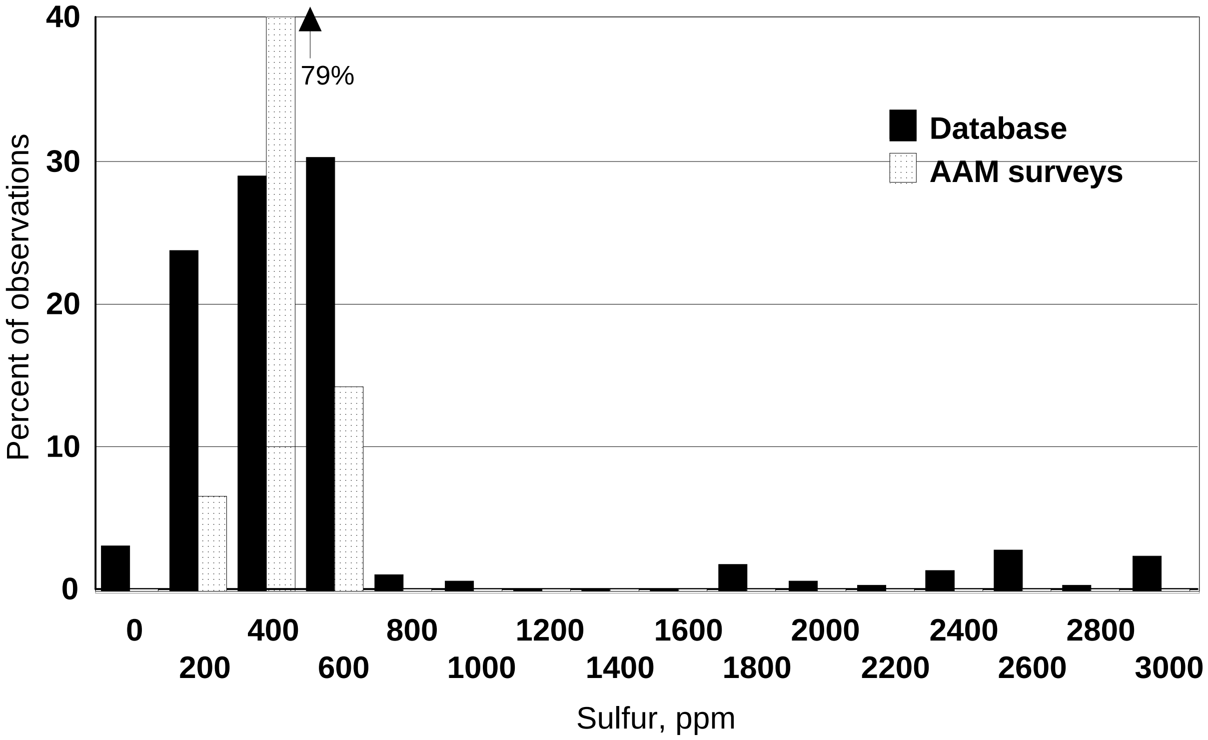


Figure II.E.1-5
Distribution of sulfur



2. Test cycles

When collecting data for use in our modeling effort for input into our database, we did not exclude data collected on any test cycle. The determination concerning which test cycles to include in which models was made subsequent to database construction. Table II.E.2-1 summarizes the number of observations in our database for each of the test cycles included in our modeling. Only observations with a measured NOx value are included in this table, though some of the observations may be missing measurements for one or more fuel property.

Table II.E.2-1
Database observations by test cycle

Test cycle	Observations	% of observations
FTP composite	401	25
FTP hot start	762	48
R49 13-mode	350	22
AVL 8-mode	87	5
All cycles	1600	100

3. Model years

Categorizing the data in our database according to the model year of the engines might provide a convenient means for applying a resulting regression model to the in-use fleet. However, we determined that defining technology groups based on such engine parameters as type of injection, rated speed, and injection control was a more appropriate way to investigate the impact of fuel properties on emissions. Still, it is instructive to examine the distribution of model years in our database and to compare them to the expected distribution of model years for a current (2002) fleet. Table II.E.3-1 provides a summary of the model years in our database and the expected in-use distribution based on MOBILE6 input data.

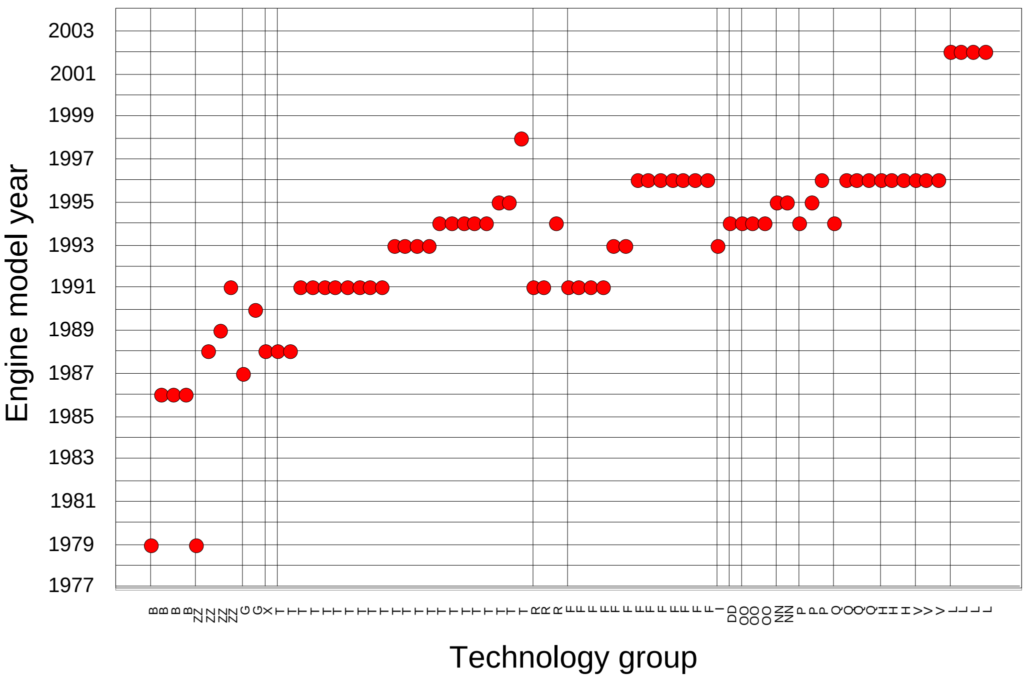
Table II.E.3-1
Model year distribution

Model year	Engines in database	Percent of engines in database	Percent of engines for 2002 fleet
1983 & prior	2	2.7	4.2
1984 - 1987	4	5.5	4.4
1988	4	5.5	1.6
1989	1	1.4	1.9
1990	1	1.4	2.3
1991	15	20.5	2.7
1992	0	0.0	3.2
1993	7	9.6	3.7
1994	12	16.4	4.4
1995	5	6.8	5.2
1996	17	23.3	6.1
1997	0	0.0	7.2
1998	1	1.4	8.5
1999	0	0.0	10.1
2000	0	0.0	11.9
2001	0	0.0	14.1
2002[†]	4	5.5	8.4

[†] All EGR-equipped engines are assumed to represent 2002 and later model years.

It is also helpful to see how our technology groups correlate with model years. Figure II.E.3-1 provides this comparison.

Figure II.E.3-1
Model years for each technology group



Section III How Was The Data Analyzed?

As mentioned previously, the goal of this study is to produce a set of correlations which predict the relative change in diesel engine emissions as a function of diesel fuel properties. We also desired to use as much of the relevant data as possible. To accomplish these goals, we applied a wide variety of regression techniques to the data described in the previous section. In this section, we first describe the fuel properties we investigated, followed by a description of the various analytical techniques which were applied to the data. Then, we present the final model for each pollutant, and show the predicted effects of changes in specific fuel properties on emissions of these pollutants.

A. Fuel terms permitted in model

There are a wide variety of fuel properties that can be used to describe diesel fuel. Some are compositional (e.g. aromatics or oxygen content), some are physical (e.g. distillation properties), and some are combustion/chemical in nature (e.g. cetane). Many of these fuel properties are interrelated, as when changes in composition also affect the physical or chemical properties of the fuel. One possible list of diesel fuel properties is given in Table III.A-1.

Table III.A-1
Diesel fuel properties

Cetane number
Cetane index
Cetane improver type
Additives (defoamers, etc.)
IBP, T10 - T90, EP
Flash point
Cloud point
Pour point
Aniline point
Copper strip corrosivity
Density
Viscosity
H/C ratio
Sulfur
Nitrogen
Oxygen
Oxygenate type
Water
Total aromatics
Monoaromatics
Polyaromatics
Ash (insolubles)
Carbon residue
Chloride
Olefins
Saturates

For the purposes of generating a model correlating diesel fuel properties with emissions of regulated pollutants, ideally one would choose the smallest set of fuel properties which provides the most precise correlation. The smaller the set of fuel properties, the greater the chance that a given study will have included them all. This is important because we want to maximize the useable data in our database, and not all studies measured all relevant fuel properties. Only those fuels in the database which include all the fuel properties that are being investigated will be included in any curve-fitting process.

As a first step in our modeling effort, we reviewed the studies listed in Appendix A to determine which fuel properties have been determined by past investigators to have the largest effect on emissions. As a result we developed a set of nine fuel properties that not only had a high likelihood for a significant correlation with emissions, but also had been measured with some regularity in the studies included in our database. The final set of fuel properties that we investigated in our modeling effort are list in Table III.A-2.

Table III.A-2
Fuel properties included in modeling effort

Natural cetane
Additized cetane
Total aromatics
Sulfur
Specific gravity
Oxygen
T10
T50
T90

One property that we believe would have been very useful is the H/C ratio. Unfortunately, very few studies in our database measured this compositional property. It may also have been useful to study mono and polyaromatics instead of total aromatics. However, as described more fully in Section III.C.1, use of these fuel properties in our modeling effort would also have significantly restricted the amount of useable data. We rejected the initial boiling point (IBP) and end point (EP) due to the less precise nature of these measurements, and with the expectation that T10, T50, and T90 together comprise a sufficient description of the distillation properties of diesel fuel. Viscosity was investigated in some studies, but did not often have a strong correlation with emissions. Indeed in the vector-based analysis conducted for the Department of Energy (discussed in more detail in Section III.B.1 below), viscosity contributed a negligible amount to the model sum of squares, and so was dropped as a model term for both NOx and PM.

B. Regression approach

The first step of the analysis was to determine what form the equations would take. We examined the distribution of emission values in our database, testing for normality. We also investigated the heteroscedastic nature of the data, examining the degree to which the variability in measurements is correlated with the magnitude of those measurements. Both investigations suggested that the use of a (natural) logarithmic transform of the emission values would help assure the applicability of the statistical methods we intended to use. The use of a log transform has been used commonly in previous fuel-focused statistical analyses conducted by other researchers. The use of a log transform also provides a benefit in terms of model simplification, since the intercept terms can be dropped when the goal of the regression is to predict the percent change in emissions in comparison to a baseline fuel. See further description in Section III.D.1 below.

We also determined that the fuel variables should be standardized in our analysis. Standardization involves calculating the mean and standard deviation for each fuel property using all of the individual values in the database that are used in the regression, subtracting the mean from every individual value of the associated fuel parameter, and then dividing this difference by the standard deviation. After the regressions have been completed, it is a trivial matter to convert back into the original fuel variables. Standardization removes the scale differences between fuel terms, allowing a more straightforward comparison of the magnitude and relative importance of the estimated fuel variable coefficients throughout the analysis. It also remove nonessential correlations between fuel terms, leading to reductions in the variances of the coefficient estimates.

We know from past experience that the effects of fuel properties on emissions are much smaller than the differences in emissions from engine to engine. To separate out the effects of fuel properties, therefore, it was necessary to include engine terms in each of our regressions (since data for only one test cycle was included in the database for any given engine). These were introduced as categorical variables in all of our models. We also included engine × fuel interaction terms for those regressions that represented fuel properties as fixed effects and engines as random effects (so-called "mixed" models based on restricted maximum likelihood). Doing so more properly accounted for the engine-by-engine variability in fuel property effects on emissions. This approach results

Instead of treating all model terms as fixed effects, we determined that it was more appropriate to represent all engine terms (whether categorical engine or engine × fuel terms) as random effects in our modeling, while continuing to treat fuel properties as fixed effects. Doing so produces regression models which are more predictive than explanatory, i.e. they can more appropriately be applied to the in-use population of diesel engines, rather than just providing an explanation of the fuel effects for the specific engines in the database. For all cases in which we were able, then, we used the proc_mix procedure in SAS in developing our final models. This procedure uses restricted maximum likelihood in place of the least-squares regressions that form the basis of "fixed" models.

Finally, we determined that only those test cycles that could be considered to be representative of the Federal Test Procedure for highway diesel engines would be included in our modeling. Test cycles were discussed in more detail in Section II.D. For the NOx and HC models, the test cycles included in our modeling were the FTP composite, FTP hot-start, Europe's R49 steady-state cycle, and the AVL 8-mode cycle. For PM, we made use of only the FTP composite and FTP hot-start data.

We examined a number of different approaches to the regression analysis. The following subsections summarize those analyses.

1. Principle Components Regressions

Principle Components Regressions (PCR) involve the conversion of the set of fuels in our database to a set of eigenvectors which, when properly weighted together, yield the original fuel set. The eigenvectors are mutually orthogonal, unlike the original fuel set, and thus provide a means for correlating individual fuel properties with emissions in such a way that important colinearities between fuel properties are preserved. If no colinearities exist in a set of data, PCR offers no advantages over more traditional regression analysis.

A recent report sponsored by the Department of Energy[11] and authored by McAdams, Crawford, and Hadder (hereafter the "McAdams analysis") promotes the use of PCR as an effective way to approach regression analysis for diesel fuel effects on emissions. When significant colinearities exist in a set of data, PCR may lead to a substantial reduction in the standard errors of the estimated fuel property coefficients, leading to a better solution. The McAdams analysis produced a model which contained only a subset of the original fuel variables considered, presumably those fuel variables which were both significant and which were correlated with one another. Since McAdams has used PCR with some success, we investigated the utility of this approach for our database.

To assess the theoretical benefit of PCR over traditional regression analysis, we calculated the Condition Number for the overall database as a measure of the colinearities it possesses. The Condition Number is equal to the square root of the largest eigenvalue divided by the smallest eigenvalue. If the Condition Number is on the order of 15, some important colinearities may exist in the data. If the Condition Number is 30 or more, severe colinearities likely exist in the data. In the database used in the McAdams analysis, the Condition Number was 13. In our current database, the overall Condition Number is 5 (though the Condition Numbers for some of the smaller technology groups were much higher). This suggests that PCR may be less advantageous for our purposes than it was for the more limited database used in McAdams' analysis.

We conducted a full principle components regression with our database for NOx, in general following the steps outlined in the DOE report (see the SwRI report[10] for details). We did this both for the database as a whole and for several technology groups that appeared to have severe colinearity problems (for instance, the data associated with technology group H had a Condition Number of 42, and the data associated with technology group B had a Condition Number of 163). After ranking the eigenvectors on the basis of statistical significance and contribution to the model sum of squares, we used the McAdams criteria of $p = 0.05$ significance and 1% contribution to the sum of squares to eliminate several eigenvectors. As a result, two eigenvectors were eliminated from the overall NOx model and three were eliminated from the overall PM model. Larger numbers of eigenvectors were eliminated from some of the technology group-specific models. We then converted back to the original set of fuel variables. Unfortunately, at this point nearly all fuel variables contributed more than 1 percent to the model sum of squares, suggesting that all fuel terms be retained in the model, according to the procedure outlined in the DOE report. Thus the PCR approach did not assist in eliminating unimportant fuel terms, and therefore did not appear to offer an advantage over more traditional regression analyses.

There are several other reasons we have chosen not to use PCR as the basis of our model at this time. First, the elimination of eigenvectors introduces some bias into the fuel property coefficients. For this reason PCR is sometimes referred to as a "biased regression approach" and is sometimes advocated primarily as a means for reducing dimensionality rather than for estimating coefficients. Second, the criteria advocated in the McAdams analysis for eliminating eigenvectors and fuel properties from the regressions is arbitrary and is not yet based on a consensus among statisticians working on these types of issues. Third, the steps for including engine variables as random effects in the context of PCR have not been developed. There are a number of other issues with PCR that, if resolved, might make PCR a more valuable tool in the future. See the SwRI report[10] for a more detailed discussion of the advantages and disadvantages of PCR.

2. Technology-group stepwise models

Because engines have such a strong effect on emissions, we felt it appropriate to consider how different types of engine technologies impact the effect of fuels on emissions. The first step was to define categories of engine technologies as described in Section II.C above.

We began our traditional regression analysis by assuming that different technologies are likely to exhibit different fuel/emission relationships. This led us to generate entirely independent models for different technology groups. In other words, we separated the data by technology group and developed regression models for the data in each group. This approach has the advantage of ensuring that any impacts that engine technology might have on the relationship between fuel properties and emissions are captured, no matter how subtle those impacts. We also determined that a forward stepwise approach to adding fuel terms into the model was appropriate in this case, since it ensured that those terms best suited to describe the data are actually included in the models. We used a $p = 0.05$ criterion for adding terms.

We encountered some limitations in the data as we developed these stepwise models. When the database was separated by technology group, some groups contained very little data. As a result, there was some suspicion that some statistically significant correlations between fuel properties and emissions for these smaller technology groups were spurious, the result of biased measurements for single test programs, the limited degrees of freedom, or some other reason. We were also faced with the fact that coefficients of zero assigned to some fuel property terms would more likely be the result of limited studies which simply did not investigate those fuel properties as opposed to having investigated them and found them to be unimportant. This meant that the smaller technology groups had fewer terms than the larger technology groups even though other non-zero fuel property coefficients might also important.

The technology groups with smaller databases also tended to have the highest condition numbers, suggestive of significant colinearities between fuel properties. In the context of a forward stepwise regression, these colinearities might reduce the descriptive power of the correlations for these smaller technology groups. For instance, the model could choose to include only one of two correlated fuel properties and provide essentially the same explanatory power as if it had chosen the other fuel property. Both models in this example would loose the link between the two collinear fuel properties. The result is that the models for these smaller technology groups might permit a user to adjusting the value of a fuel property that is not represented in the model even though it might have a significant impact on emissions.

Once the models were completed for those technology groups with sufficient data, we discovered that many of the fuel property coefficients were similar across technology groups. In the NOx models, for instance, the coefficients for distillation properties, sulfur, and oxygen were all at or near zero, while the coefficients for aromatics, natural cetane, and additized cetane exhibited only very small differences from one another. These differences were generally less than the uncertainty in the coefficients. As a result, we questioned the need for independently-generated technology group models, since this approach appeared to increase model complexity without improving its predictive power, with the additional problem that the models were more difficult to apply to the in-use fleet. We therefore decided that an approach which assumed that all technology groups exhibit the same fuel effects unless proven otherwise would be more appropriate.

3. Unified model

In an effort to promote model simplicity while still permitting engine technology to play a role in correlations between fuel properties and emissions, we developed a "unified" approach to the regressions. In this approach, forward stepwise regressions were carried out on the database as a whole, but technology group-specific fuel effects were also permitted to enter the model if significant. We also made efforts to more properly account for engine variability and the impact that such variability should have on the statistical significance of fuel property coefficients. The resulting Unified Model is the model that we are proposing in this staff discussion document as a means for predicting the impact of changes in diesel fuel properties on emissions.

We separated the process of selecting model terms from the process of estimating coefficients for those terms deemed statistically significant. The first stage was aimed at generating a collection of fuel terms that had a strong likelihood of being important elements in the final correlations. We used a fixed model in SAS because this permitted us to automate the process. To make the selection of fuel terms, we first averaged all repeat emission measurements to avoid overweighting those fuel/engine combinations that had many repeat measurements. We then used a fixed model with categorical variables for the engines to conduct a sequential forward stepwise regression, consisting of five phases. In all phases, the criterion for significance was $p = 0.05$. The five phases are described below:

1. Conduct a forward stepwise regression, allowing as candidates for entry only the nine linear fuel terms.

2. Starting with the model from Step 1, conduct another forward stepwise regression, allowing as candidates for entry only the nine squared fuel terms.
3. Starting with the model from Step 2, conduct another forward stepwise regression, allowing as candidates for entry only the thirty-six fuel×fuel interaction terms.
4. Starting with the model from Step 3, conduct another forward stepwise regression, allowing as candidates for entry only the nine technology group × linear fuel terms.
5. Starting with the model from Step 4, conduct another forward stepwise regression, allowing as candidates for entry only the nine technology group × squared fuel terms.

Up to this point, no terms were removed from the model once they were added. After phase 5, we conducted three other checks to make sure we continued into the second stage of the Unified Model with only those terms which were truly necessary. First, some terms that had been forced into the model in phase 5, which earlier had been statistically significant, ceased to be significant by the end of phase 5. These terms were dropped all at once. Second, we reviewed Mallow's Cp criterion and determined that we had begun to overfit the model in phase 5. We therefore eliminated several terms, beginning with those added in phase 5 and working backwards, until Cp was equal to the number of terms (indicating a balance between over and under-fitting). Finally, we reviewed the variance inflation factors for terms in the model to determine if any of the terms might be problematic. We used a criterion of 100, which would indicate that a given term exhibited an extreme correlation with other model terms and was therefore unnecessary. Once this first stage of the Unified Model was completed, we were assured that the resulting model would only be as complex as necessary to include whatever nonlinear or technology group-specific effects were important.

We did not place any restraints on whether a technology group-specific term could enter the model in the context of the sequential stepwise regression, other than statistical significance. However, it may have been appropriate to consider the amount of data in each technology group in this process. For instance, a number of technology groups consisted of only a single engine. It may be appropriate to establish some type of criteria based on the amount of data in a given technology group which would determine whether our Unified Model approach would permit that technology group to have its own fuel effects. We did not investigate such an approach, but we request comment on how such criteria could be established and used.

The second stage of the Unified Model made use of the proc_mix procedure in SAS. Since this procedure does not produce estimates of the r^2 values for the models, we can only provide r^2 values for the models resulting from the sequential stepwise regression. These values are shown in Table III.B.3-1.

Table III.B.3-1
R squared values after sequential stepwise regressions

Model	R^2 value
NOx	0.996
PM	0.991
HC	0.953

In the second stage of the Unified Model, we more fully accounted for engine variability. We were then able to determine if the fuel terms surviving the first stage of the Unified Model remained statistically significant, and we could estimate the coefficients for those fuel terms. In this stage, the full dataset, including all repeat measurements, is used in the SAS procedure proc_mix with all the terms identified in the first stage of the analysis. Engine × linear fuel interaction terms are added to the model in addition to the engine intercept terms, all of which are identified as random effect terms. Technology group intercepts are also added for those technology groups actually present as specific terms in the model. These intercepts were forced into the model regardless of their statistical significance to maintain hierarchy. After the proc_mix procedure was run, terms that were not significant at the $p = 0.05$ level were dropped, beginning with technology group terms and working back towards the linear common fuel terms. After each set of insignificant terms was dropped, the coefficients and significance were recalculated and the process repeated until all terms in the model were significant. This approach again ensures that the model will be as simple as possible while still permitting technology group-specific terms to remain in the model if they are important. Once this backwards stepwise regression was completed, the regressions were complete.

The final Unified Models for NOx, PM, and HC were in standardized variable form, and contained all technology group terms as adjustments from the common linear and squared fuel terms. To make the equations more user-friendly, the fuel variables were first unstandardized. The common terms (applicable to all technology groups) and adjustments for specific technology groups are given in Tables III.B.3-2, III.B.3-3, and III.B.3-4 for NOx, PM, and HC respectively.

We then generated independent equations for each technology group by adding the technology group adjustments to the common fuel terms. This process resulted in a polynomial function of fuel variables for each of the technology group-specific models and for the default model. Since the emission measurements were rendered as the natural log of emissions during the regression analysis, the equations were converted into a more useable form by rendering emissions as a function of the exponential of the polynomials. The final result of these manipulations was a set of equations for each pollutant which provided emissions in g/bhp-hr as a function of the exponential of a polynomial function of fuel properties. The coefficients for the fuel properties are given in Tables III.B.3-5, III.B.3-6, and III.B.3-7 for NOx, PM, and HC respectively. Note that the "Default" model applies to all technology groups except for those that have their own technology group-specific model.

Table III.B.3-2 Unstandardized coefficients for NOx model with technology group adjustments

	Common terms	Tech group B adjustments	Tech group L adjustments	Tech group R adjustments	Tech group X adjustments	Tech group H adjustments
Intercept	0.50628	0.46541	-0.64011	-0.05788	5.2757	-0.41201
Natural cetane	0	0.005553	0	0	0	0
Cetane difference	-0.002779	0.007378	0.003951	0	0	0
Aromatics, vol%	0.002922	0	0	0	0	0
Sulfur, ppm	0	0	0	0.0001018	0	0
Specific gravity	1.3966	0	0	0	0	0
T50, ^{o}F	-0.0004023	0	0	0	-0.0214077	0.0008815
T50 squared	0	0	0	0	0.00002139	0

Table III.B.3-3 Unstandardized coefficients for PM model with technology group adjustments

	Common terms	Tech group X adjustments	Tech group ZZ adjustments
Intercept	-3.75781	3.44171	-3.77928
Natural cetane	-0.004521	-0.122579	0
Natural cetane squared	0	0.001206	0
Cetane difference	-0.04825	0	0
Aromatics, vol%	0.002157	0	0
Sulfur, ppm	0.00008386	0	0
Specific gravity	2.3708	0	0
Oxygen, wt%	-0.07193	0	0
T90, ^{o}F	0	0	0.007480
Natural cetane × cetane difference	0.001009	0	0

Table III.B.3-4 Unstandardized coefficients for HC model

	Common terms
Intercept	5.32059
Natural cetane	-0.1875
Natural cetane squared	0.001571
Cetane difference	-0.1880
T10, ºF	-0.0009809
T50, ºF	-0.002448
Natural cetane × cetane difference	0.003507

Table III.B.3-5 Final coefficients for NOx model

NOx (g/bhp-hr) = exp(intercept + a × natural cetane + b × cetane difference + ⋯)

	Default	Tech group B	Tech group L	Tech group R	Tech group X	Tech group H
Intercept	0.50628	0.97169	-0.13383	0.44840	5.78198	0.09427
Natural cetane	0	0.005553	0	0	0	0
Cetane difference	-0.002779	0.004599	0.001172	-0.002779	-0.002779	-0.002779
Aromatics, vol%	0.002922	0.002922	0.002922	0.002922	0.002922	0.002922
Sulfur, ppm	0	0	0	0.0001018	0	0
Specific gravity	1.3966	1.3966	1.3966	1.3966	1.3966	1.3966
T50, ºF	-0.0004023	-0.0004023	-0.0004023	-0.0004023	-0.02181	0.0004792
T50 squared	0	0	0	0	0.00002139	0

Table III.B.3-6 Final coefficients for PM model

PM (g/bhp-hr) = exp(intercept + a × natural cetane + b × cetane difference + ⋯)

	Default	Tech group X	Tech group ZZ
Intercept	-3.75781	-0.31610	-7.53709
Natural cetane	-0.004521	-0.1271	-0.004521
Natural cetane squared	0	0.001206	0
Cetane difference	-0.04825	-0.04825	-0.04825
Aromatics, vol%	0.002157	0.002157	0.002157
Sulfur, ppm	0.00008386	0.00008386	0.00008386
Specific gravity	2.3708	2.3708	2.3708
Oxygen, wt%	-0.07193	-0.07193	-0.07193
T90, ^{o}F	0	0	0.007480
Natural cetane × cetane difference	0.001009	0.001009	0.001009

Table III.B.3-7 Final coefficients for HC model

HC (g/bhp-hr) = exp(intercept + a × natural cetane + b × cetane difference + ⋯)

	Default
Intercept	5.32059
Natural cetane	-0.1875
Natural cetane squared	0.001571
Cetane difference	-0.1880
T10, ^{o}F	-0.0009809
T50, ^{o}F	-0.002448
Natural cetane × cetane difference	0.003507

Note that the default NOx model contains no term for natural cetane. This is an unexpected result, and warrants further attention. There was also some expectation that natural cetane and additized cetane would produce more similar effects on emissions, based on several studies that examined this particular issue. These issues are discussed more fully in Section VII.B.

C. Sensitivity analyses

There are many different fuel properties that could be chosen as independent variables when investigating potential correlations between fuel properties and emissions. There are also many different fuel term forms that can be investigated, such as squared and interactive fuel terms. The terms and term forms we used in our model development were chosen on the basis of a preliminary review of the studies from which the data in our database was derived. There are alternatives that we investigated or intended to investigate that might be important elements in a model correlating diesel fuel properties with emissions. This section addresses some of those alternatives.

1. Monoaromatic versus polyaromatic effects

A number of studies investigated the emission impacts of subcategories of aromatic compounds. In these studies, the most typical approach was to separate monoaromatic compounds (hydrocarbons containing a single benzene ring) from polyaromatics (hydrocarbons containing more than one benzene ring). A smaller set of studies made further distinctions between mono, di-, and tri-aromatic compounds. In the studies that actually measured these subcategories of aromatics, some actually made efforts to control the test fuel levels of one subcategory of aromatics separately from another subcategory of aromatics. In most cases, the polyaromatics were specifically controlled while the monoaromatics were uncontrolled.

These studies offered evidence that different types of aromatic compounds may have different impacts on emissions, particularly for PM. Some studies, such as the ACEA study, also concluded that mono and polyaromatic compounds may exhibit different effects for NOx. On this basis, then, it would have been reasonable to investigate these potential effects in our modeling effort by including monoaromatic and polyaromatic terms instead of the single total aromatics term.

In our modeling approach, the first phase involves a sequential stepwise regression in the context of the SAS procedure proc_reg. When we specify the selection of fuel properties that are candidates for entry into the model during the stepwise regression, this procedure makes use of only that data that contains all of the candidate fuel properties. For instance, since we determined that T50 would be a candidate for entry into the model, SAS made use only of data that included a non-blank T50 value, resulting in a loss of approximately 10% of the data in our database. If we had included monoaromatic and polyaromatic terms in our stepwise regression, we would have lost over 50% of the data in our database. This is a significant amount of data to lose, and the model could potentially have exhibited different fuel property/emissions correlations as a result. Thus we determined that it was more reasonable to include only a total aromatic term for our draft model than to lose 50% of the available data.

Ideally, the emission effects of the sum of mono and polyaromatics would be based on the entire database, while the separate effects for mono and polyaromatics would be based on the subset of the data that actually contains measurements for these two fuel properties. Unfortunately, a methodology for doing this is currently unavailable. We request comment on whether and how to include the separate effects of monoaromatics and polyaromatics in our modeling approach.

2. Correlating additized cetane effects with baseline natural cetane

There was some expectation during our model development that the effects of additized cetane on emissions would diminish as the base cetane number increased for the fuel to which cetane improver was added. In other words, for a fixed cetane difference value, the impact on emissions would be a function of the natural cetane value of the fuel. The most straightforward way to account for the possibility of this effect is to include an interactive term of the form natural cetane × cetane difference. Since our Unified Model included all possible fuel-by-fuel interactions as candidates in the sequential stepwise stage of model development, no special effort was necessary to account for this particular interactive effect.

As can be seen by the coefficients in Tables III.B.3-5 through III.B.3-7, the PM and HC models do in fact include natural cetane × cetane difference terms. However, no such term arose in the NOx model. Earlier investigations of technology group-specific stepwise models indicated that this interactive term was not significant for the largest technology group T, but was significant in the technology group F+DD model (a model based on the combination of data from technology groups F and DD, which differ from one another only in the existence or absence of an oxy catalyst). But for the database as a whole, it appears that a natural cetane × cetane difference term is not an important element in the way in which additized cetane affects NOx emissions.

D. Incorporation of baseline fuel

The model presented in this staff discussion document must be used in connection with MOBILE model output in order to estimate the inventory impacts of changes to diesel fuel. The most straightforward way to do this is to calculate a percent change in emissions based on a given change to diesel fuel properties using the model presented in this discussion document, and then to apply this percent change to the emissions estimated by MOBILE. This approach requires that we define a baseline fuel from which changes can be assessed.

The baseline fuel incorporated into our model represents the current nationwide, annual average highway diesel fuel. We used data from recent surveys conducted by the Alliance of Automobile Manufacturers (AAM). We averaged the annual average fuel properties across years

1995 through 2000. Since our model makes use of natural cetane and cetane difference rather than total cetane, we needed to estimate the portion of the total cetane number that resulted from the use of cetane improver additives. To do this, we used two independent approaches:

> *Approach #1*: The AAM surveys include estimates of the amount of cetane improver additive in the fuels tested. We used the following correlation from SAE paper number 972901 to convert these amounts into an equivalent increase in cetane number:
>
> $$CNI = 0.16 \times CN^{0.36} \times G^{0.57} \times C^{0.032} \times \ln(1 + 17.5 \times C)$$
>
> Where:
>
> CNI = Predicted cetane number increase due to an additive
> CN = Base cetane number
> G = Fuel API gravity
> C = concentration of additive in vol%
>
> *Approach #2*: The AAM surveys also include calculated cetane index values. Cetane index values are often used as surrogates for cetane number if the latter is missing. However, cetane index values cannot account for the existence of a cetane improver additive, and so can only be used to estimate unadditized or "base fuel" cetane number values.
>
> Recent analyses by Ethyl corporation, confirmed by our own analysis of unadditized fuels in the AAM database, indicates that cetane index does not have a 1:1 correlation with natural cetane number as formerly believed. Instead, the following equation appears to provide a much more precise relationship:
>
> $$\text{Natural cetane number} = 1.154 \times \text{Cetane index} - 9.231$$
>
> The AAM survey results included measurements of both cetane index and cetane number. The existence of a cetane improver additive will cause cetane index and cetane number to differ by an amount greater than the difference suggested by the above equation. This difference is indicative of the increase in cetane number due to the existence of the additive. Thus in association with the equation above, we were able to calculate the increase in cetane number that was due to the addition of a cetane improver additive.

The results for approaches 1 and 2 were very similar. We therefore averaged the results from these two approaches to generate baseline natural cetane and cetane difference values. The final baseline fuel properties for highway diesel fuel are shown in Table III.D-1.

Table III.D-1
Baseline Fuel Properties

Property	Value
Natural cetane number	44.1
Cetane number increase due to additives	0.8
Aromatics, vol%	34.4
Specific gravity	0.85
Sulfur, ppm	333
Oxygen, wt%	0
T10, °F	422
T50, °F	505
T90, °F	603

We modified the model equations so that they would automatically produce estimates of the percent change in emissions based on a change from the baseline fuel. Since the equations were based on regressions on the natural log of emissions, they could be represented in the following form:

$$\text{Emissions (g/bhp-hr)} = \exp(f(\text{cetane, aromatics, etc.}))$$

where f is a polynomial function of diesel fuel properties. The percent change in emissions is therefore

$$\%\ \text{change in emissions} = [\exp(f(\text{target fuel}) - \exp(f(\text{baseline fuel})] / \exp(f(\text{baseline fuel}) \times 100\%$$

where the target fuel is the fuel whose properties are under consideration, and the baseline fuel is that given in Table III.C.1-1. Note that any constants in the function f will cancel out of the above equation. This equation can be rearranged to:

$$\%\ \text{change in emissions} = [100 / \exp(f(\text{baseline fuel})] \times \exp(f(\text{target fuel}) - 100$$

The incorporation of the baseline fuel properties into the above equation need be done only once, so that the above equation can be represented as:

$$\%\ \text{change in emissions} = C \times \exp(f(\text{target fuel})) - 100$$

The constant C is called a “transformation constant” since it transforms the original equations, giving emissions in terms of g/bhp-hr, into equations that give the percent change in emissions with respect to the baseline fuel. The function f is simply that given in Tables III.B.3-5, III.B.3-6, and III.B.3-7 for NOx, PM, and HC, respectively. However, we can ignore the intercepts for the regression equations since they cancel out when one is calculating a percent change in emissions. We calculated the constant C for every equation in our model (minus the intercepts) using the baseline fuel properties in Table III.D-1. These transformation constants are shown in Table III.D-2 for the Unified Model equations.

Table III.D-2
Model Transformation Constants

Model	Constant C		
	NOx	PM	HC
Default	33.883	14.735	98035
Tech group B	26.366	n/a	n/a
Tech group L	33.776	n/a	n/a
Tech group R	32.753	n/a	n/a
Tech group X	7175.0	314.57	n/a
Tech group H	21.710	n/a	n/a
Tech group ZZ	n/a	0.16198	n/a

The model equations with the above transformation constants provide a means for estimating the impact of fuel property changes on emissions for all vehicles in the current fleet.

E. Extrapolation and valid ranges

The applicability of any model to in-use fuels is limited by the distribution of fuel properties in the database on which the model is based. It is also important to take into account expected future fuels which may be cleaner than current fuels. Extrapolation can be used to extend model equations into regions of the multi-dimensional fuel property space that are not well represented by the database. If extrapolation cannot be justified, valid range limits may need to be assigned to the models. Valid range limits define the range of fuel properties within which the model equations can be used, and outside of which the predictions offered by the model equations are considered speculative and therefore not trustworthy.

Section II.E presented ranges of fuel properties for fuels in our database through distribution plots. Included in those figures were summaries of in-use fuels surveys. For the most part, the data in our database does provide significant overlap with in-use fuels data, suggesting that our model can be used to evaluate most in-use fuels. In addition, the database actually contains many fuels which are generally cleaner than those found in-use. Since the primary use of the model will be to evaluate the emission benefits of cleaner fuels, this fact is an advantage for our model.

We can delineate the region within which the predictions from our model can be considered trustworthy by examining the range of fuel property values in our database. As one approaches the edges of the fuel property dataset (e.g. very high or very low aromatics values), the confidence we have in the model's predictions decreases. Thus one way to define the valid range limits of the model is to determine high and low values for each fuel property that encompass a majority of the data.

Using the subset of the database upon which the NOx model was based, we determined the two limiting values for each fuel property that encompassed 98 percent of the data. Thus 1 percent of the data lay above the high limit, and 1 percent of the data lay below the low limit; the valid range limits are thus defined by the percentile criteria 1 and 99. These results are shown in Table III.E-1.

Table III.E-1
Valid range limits

Fuel property	Lower limit	Upper limit
Natural cetane	38	66
Cetane difference	0	17
Aromatics, vol%	3	48
Sulfur, ppm	0	3000
Specific gravity	0.78	0.88
Oxygen, wt%	0	3.5
T10, °F	340	525
T50, °F	425	585
T90, °F	515	685

We believe that the Unified Model should not be used to evaluate fuels outside the range of fuel properties given in Table III.E-1, and one should use caution when evaluating fuels near the valid range limits. Note that the oxygen limit of 3.5 wt% should also be combined with a 20 vol% limit on fuel oxygenate content, consistent with the limit we used in assembling the database.

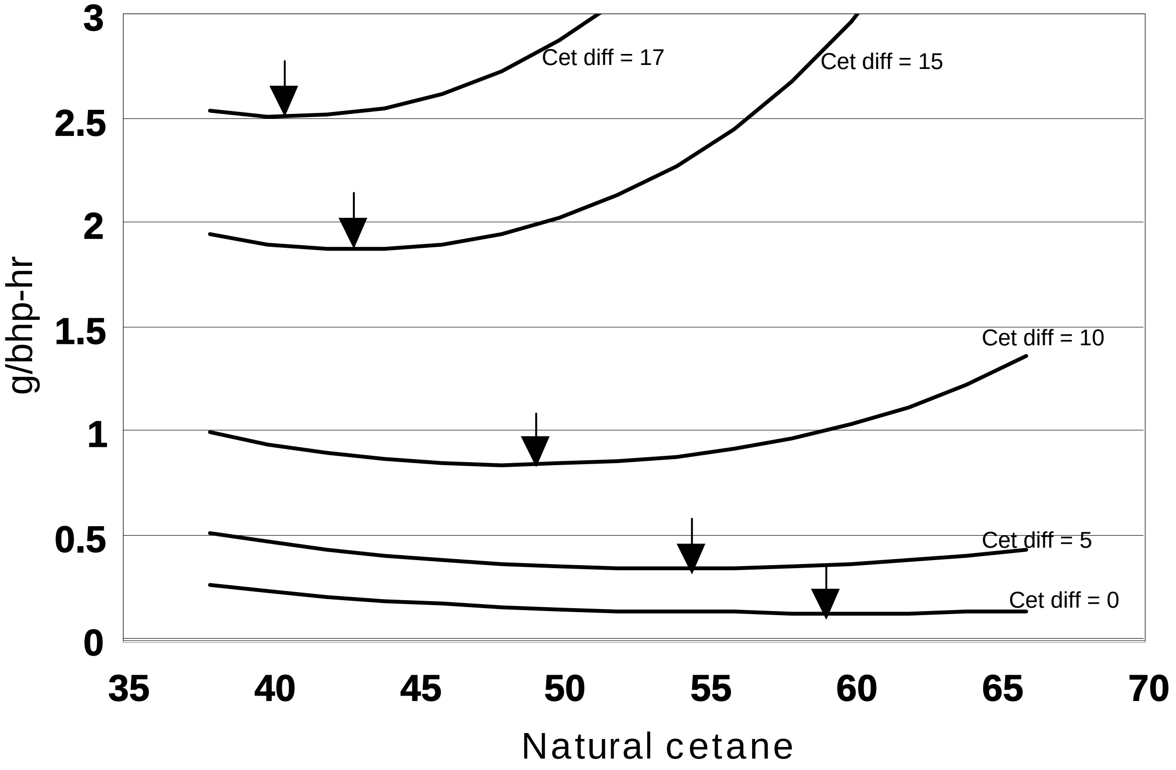
We do not believe it is appropriate to extrapolate the model into regions of the fuel property space that lie outside the valid range limits. The ranges defined by the values in Table III.E-1 are at least as wide as current in-use fuels, and in some cases are actually wider, so that fuels whose properties lie outside of our valid range limits would be unlikely. In addition, our percentile criteria of 1 and 99 percent capture the greatest possible amount of data, with the result that the model equations could easily be unrepresentative of fuel property effects on emissions if used outside the valid range limits. Even so, there may be cases in which a fuel with extremely high or low fuel properties must be evaluated for emission impact trends, if not absolute emission effects. For these cases we recommend that the equations be "flat-lined" outside the valid range limits. In other words, the emission effects predicted by the model at the valid range limits should be used for any cases where a fuel property exceeds the valid range limit.

Note that, notwithstanding the valid range limits, the Unified Model should not be used to evaluate biodiesel, diesel/water emulsions, or other alternative fuels. Fischer-Tropsch fuels are not categorically excluded from the model (indeed the database contained several Fischer-Tropsch fuels), but they should still be considered in the context of the valid range limits.

Among all the default models, there are only two cases in which nonlinear fuel terms produce turnover effects within the valid range limits. Both involve the natural and additized cetane terms, and both are cases in which we believe the model should be amended to prevent counterintuitive emission effect predictions which are simply artifacts of our selection of fuel terms. To amend the models, we have implemented flat-line extrapolation.

In the default HC model, the existence of a squared term for natural cetane means that HC emissions are predicted to decrease with increasing natural cetane, until a minimum (mathematical extrema) is reached, after which the model predicts that HC emissions will *increase* with increasing natural cetane. In addition, the default HC model includes an interactive term for natural cetane × cetane difference, which forces the minimum point to vary. The effects of these nonlinear terms can be seen in Figure III.E-1. The arrows indicate the location of the minimum emissions values.

Figure III.E-1
Floating turnovers in default HC model



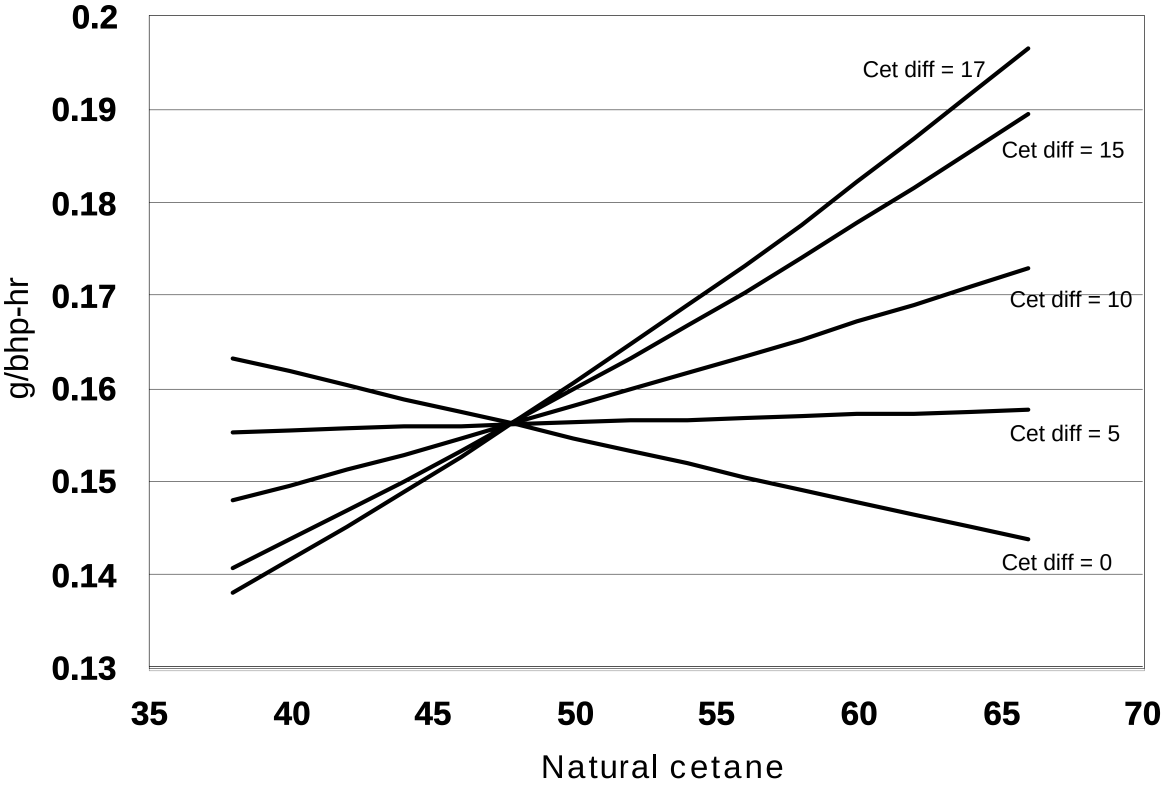
Based to our stepwise modeling for individual technology groups, we would expect HC emissions to decrease as natural cetane increases. Therefore, we have determined that the predicted HC emissions should be held constant for any increases in natural cetane number above the mathematical extrema. Setting the first partial derivative for natural cetane equal to zero in the default HC model, we have derived an equation that calculates the location of the mathematical extrema as a function of the cetane difference. This equation is:

"Turnover" point for natural cetane = -1.11598 × CETDIFF + 59.6493

In practice, the natural cetane value that is entered into the default HC model should never be higher than the value calculated with the above equation.

The default PM model also exhibits a turnover problem for natural cetane, but in this case the turnover in question is associated with the slope of the entire curve, not just one point on the curve. The problem is illustrated in Figure III.E-2.

Figure III.E-2
Turnover effects in default PM model



A similar graph can be shown for cetane difference, in which the slope of the curve is a function of the natural cetane number.

Once again we believe, based on stepwise regressions with individual technology groups, that the primary trend should be for PM emissions to decrease as natural cetane or cetane difference increases. Therefore, we have determined that:

1. The predicted effect of a change in natural cetane on PM emissions should be zero whenever the cetane difference value exceeds 4.48 (the value beyond which the natural cetane slope changes from negative to positive).

2. The predicted effect of a change in cetane difference on PM emissions should be zero whenever the natural cetane value exceeds 47.81 (the value beyond which the cetane difference slope changes from negative to positive).

In practice, this means that the cetane difference value that is entered into the default PM model should be 4.48 if the actual cetane difference value is higher than 4.48 *and* the actual natural cetane value is higher than 47.81. Likewise the natural cetane value that is entered into the default PM model should be 47.81 if the actual natural cetane value is higher than 47.81 *and* the actual cetane difference value is higher than 4.48.

F. Summary of emission effects exhibited by equations

The original intention of developing a model correlating diesel fuel properties with emissions was to ensure that the specific benefits claims for clean diesel fuel in the Texas State Implementation Plan were accurate. Given the nature of Texas' clean diesel fuel program, we expect that fuel currently being sold in California is the best representation of what fuel in Houston and Dallas is likely to look like under their clean diesel fuel program. Therefore, we can examine the impacts that current California diesel fuel has on emissions according to our model as a way of estimating the benefits of Texas' program.

The average properties of current California diesel fuel were taken from surveys conducted by the Alliance of Automobile Manufacturers from 1995 through 2000, to be consistent with those for the baseline fuel as described in Section III.D-1 above. We were forced to use the survey results from one city, Los Angeles, since this is the only Californian city sampled in the AAM surveys. Also similar to the baseline fuel, we were forced to estimate the contribution that cetane improver additives make to the total cetane number of the average Californian diesel fuel. The results are shown in Table III.F-1.

Table III.F-1
Average California Fuel Properties

Property	Value
Natural cetane number	47.9
Cetane number increase due to additives	4.4
Aromatics, vol%	21.9
Specific gravity	0.837
Sulfur, ppm	130
Oxygen, wt%	0
T10, °F	418
T50, °F	502
T90, °F	613

We can input the fuel properties from Table III.F-1 into our default models to predict the impacts that the Texas clean diesel fuel program is likely to have on emissions from the heavy-duty fleet. These results are shown in Table III.F-2 for a "current" fleet (i.e. assuming EGR-equipped engines have not yet entered the fleet).

Table III.F-2
Percent reduction in emissions for California diesel fuel

NOx	PM	HC
6.2	8.5	19.4

We can also use our equations to estimate the emissions impacts of discrete changes in specific diesel fuel properties. We have done this for each of the fuel properties that are represented in our model. In each case, the change was made to only one fuel property at a time, and was made relative to the baseline fuel defined in Table III.D-1. Colinearities between fuel properties were not taken into account. The results of these changes are shown in Table III.F-3 for a "current" fleet.

Table III.F-3
Predicted percent emission reductions for discrete changes in fuel properties
(all values relative to baseline fuel)

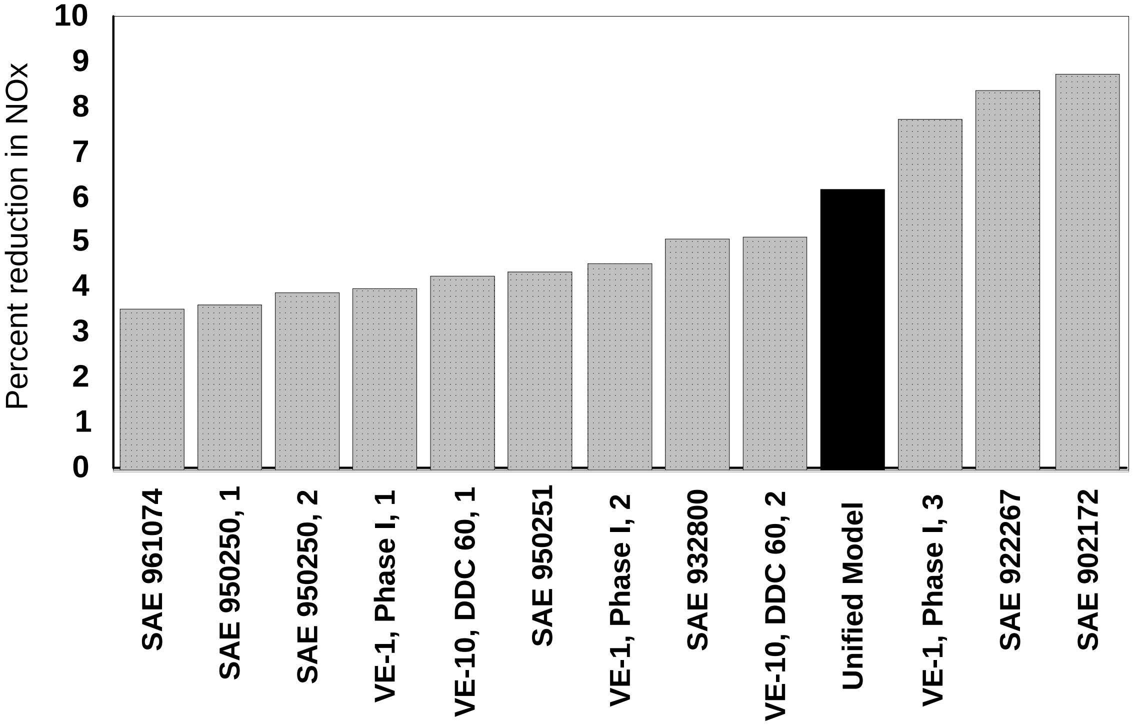
	NOx	PM	HC
Increase natural cetane by 5 numbers	0	1.8	17.4
Increase additized cetane by 5 numbers	1.4	1.9	15.3
Decrease aromatics by 10 vol%	2.9	2.1	0
Decrease specific gravity by 0.05	6.7	11.2	0
Decrease sulfur by 100 ppm	0	0.8	0
Increase oxygen by 1 wt%	0	6.9	0
Decrease T10 by 10 °F	0	0	-1.0
Decrease T50 by 10 °F	-0.4	0	-2.5
Decrease T90 by 10 °F	0	0	0

G. Comparisons to other emission models

As described in Section III.A, the different approaches that we investigated for generating regression equations did not appear to produce dramatically different results. But this fact may not be sufficient to conclude that our Unified Model provides reasonable predictions of fuel property effects on emissions. Therefore, it seemed prudent to compare predictions from our model to those from independent models created and published previous to this staff discussion document.

We used the survey results for fuel sold in Los Angeles to make this comparison (Table III.F-1). We input these fuel properties into a number of regression models for NOx developed by the authors of several different studies. Note that data from all of these studies were used in the development of the Unified Model. Figure III.G-1 shows the result.

Figure III.G-1
Comparative NOx predictive effects for Los Angeles diesel fuel



As this Figure shows, the predictions from our Unified Model compare favorably with those based on equations from other sources. Note that most of the other models do not contain a full complement of fuel properties, and many contain only two. Since the NOx benefits of fuel sold in Los Angeles arise from several different fuel properties, models with fewer terms might not predict the full benefit. In addition, the above Figure gives no indication of the amount of data each study contributed to our database, so drawing quantitative conclusions about the reliability of our model from this Figure would be premature.

In 1998, MathPro Inc. and Energy and Environmental Analysis Inc. jointly produced a report for the State of Arizona in which they summarized their analysis of the impacts of changes in diesel fuel on emissions[12] ("the MathPro report"). In similar fashion to our own analysis, the authors collected data from several different studies and conducted a regression analysis. Their database included 15 studies (in contrast to the 35 studies in our database), all of which contained transient cycle (FTP) test data. Although not as comprehensive as our own database, the MathPro model should provide a point of comparison to ensure that our own model is reasonable.

We chose a selection of changes in fuel properties consistent with those used in Table III.F-3 to determine how the predicted effects from our Unified Model and the MathPro model compared. The results are shown in Table III.G-1.

Table III.G-1
Comparison of Unified Model and MathPro model

	% reduction in NOx		% reduction in PM		% reduction in HC	
	Unified Model	MathPro model	Unified Model†	MathPro model	Unified Model†	MathPro model
Increase natural cetane by 5 points	0	1.4	1.8	1.8	17.4	20.1
Increase additized cetane by 5 points	1.4	1.4	1.9	1.8	15.3	20.1
Lower aromatics by 10 vol%	2.9	0.2	2.1	5.2	0	-1.4
Lower specific gravity by 0.05	6.7	0	11.2	10.3	0	0
Lower sulfur by 100 ppm	0	0.2	0.8	0.3	0	0

† "Best engineering models" were from the Mathpro report were used in this analysis

In every case, the Unified Model and the MathPro model predict consistent directional changes in emissions for a given change in fuel properties. In most cases, the magnitudes of the predicted effects are also very similar. There are, however, some differences that could not be explained without a more thorough comparison of the two databases. For instance, the Unified Model appears to predict larger changes in NOx for reductions in aromatics and specific gravity. Even if the colinearities between these and other fuel properties are taken into account, the MathPro model still predicts NOx benefits one-third the size of the benefits predicted by the Unified Model. The Mathpro model also counter intuitively predicts an increase in HC emissions when aromatics are lowered, a fact that is addressed directly in the MathPro report.

We request comment on the Unified Model in comparison to the MathPro model. Specifically, whether any of the following had a significant influence on the model coefficients:

- The inclusion of steady-state data in our database
- Differences in statistical methodology
- Differences in the selection of fuel property terms to permit in the models
- The distribution of engine technologies in the two databases
- The degree to which studies in each database decorrelated fuel properties

Section IV How Should The Model Be Used?

A. Technology group weightings

Our final model resulted from a regression approach that yielded one "default" model for each pollutant which applies to most of the fleet, and several technology group-specific models. To apply the fuel/emission effects exhibited by our final model to the entire in-use fleet, therefore, each of the technology group-specific models should be weighted according to the fraction of the in-use fleet that is represented by those technology groups. Ideally, this would require a detailed description of the in-use fleet that would include all of the engine parameters listed in Table II.C-1. Unfortunately, this type of description is not readily available. However, we did compile recent certification data that included rated speed, type of aspiration, horsepower, engine displacement, and the type of injection control. From this information we were able to determine which of our technology group-specific models would be expected to be important additions to the fleet-wide effects predicted by the default models.

We used 1998-1999 certification data for diesel engines in this analysis, as this information was readily available. We had separate databases available for highway and nonroad engines. The certification data available did not include sales, but only listed certifications by engine family. Thus this information enabled us only to roughly estimate the percent of recent engine sales which would be expected to fall into specific technology groups. This analysis yielded the results shown in Table IV.A-1 for those technology groups having their own model.

Table IV.A-1
Percent of selected technology groups in certification database

Technology group	Highway engines	Nonroad engines
B	0	5
H	0	1
L	0	0
R	0	0
X	9	16
ZZ[†]	0	0

[†] All naturally aspirated engines also had indirect injection, and so were categorized as technology group X.

Two-stroke engines (technology group B) are not separated from 4-stroke engines in either the highway or nonroad certification database. However, we were able to use the current version of EPA's NONROAD model to estimate that only 5% of the current nonroad fleet is 2-stroke engines. For highway vehicles, we know that the only 2-stroke engines sold in recent years were produced by Detroit Diesel Corporation, who stopped production of these engines in 1997.

From this recent data, it is clear that the technology groups which have their own model represent a rather small portion of current engine certifications and presumably sales. Although we don't have a straightforward means for estimating the contribution that these technology groups make to the full in-use fleet, we can surmise from this certification data that the fraction is small and will continue to decline over time. This conclusion may not apply to technology group X (indirect engines), since they appear to be a not insignificant portion of current sales, or technology group L (EGR-equipped engines), which are expected to increases in numbers in the future. Aside from these two exceptions, discussed more fully below, it appears appropriate to apply the effects exhibited by our default models for NOx, PM, and HC to the in-use fleet and to assume that the emission effects exhibited by technology group-specific models can be dismissed until the in-use fleets can be better characterized.

As can be seen from the values in Table IV.A-1, indirect engines may represent a potentially not insignificant portion of the in-use fleet for both highway and nonroad. In our Unified Model, there is an independent equation for technology group X for both NOx and PM. However, our final NOx model for technology group X differs from the default model only in terms of the effect of T50 on emissions. The slope of the T50 effects on NOx in the region of national average fuel properties is essentially identical for the default and technology group X models. As a result, we believe we can safely dismiss the technology group X model for NOx and instead use only the default NOx model when making estimates of emissions impacts for the both the highway and nonroad in-use fleets.

For PM, the technology group X model differs from the default PM model in the natural cetane effect. Natural cetane has only a small impact on PM emissions in the default PM model relative to the effects of other fuel properties; specific gravity has by far the dominant impact. Thus any weighting of the default and technology group X models for PM is unlikely to differ substantially from the effects of the default model alone. For instance, if a weighting factor of 0.09 was applied to the technology group X equation and a weighting factor of 0.91 was applied to the default equation consistent with the highway certification results in Table IV.A-1, California-like fuel[i] would produce the PM reductions shown in Table IV.A-2.

Table IV.A-2
Impacts of technology group X on percent reduction in PM emissions

Default model	Default and technology group X models
8.5	8.8

Even though we used a weighting based on certification data in this example, we do not currently believe that we can confidently establish a weighting factor for technology group X in the PM model for either the highway or nonroad in-use fleets. We will continue to investigate assigning a

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[i] Based on fuel properties in Table III.F-1

weighting factor to the technology group X model for PM. In the meantime, we propose that the default PM model be used.

Finally, we expect EGR-equipped engines to become a larger portion of the highway fleet in the near future, and thus it seems prudent to include the NOx emission effects predicted by technology group L in any estimate of fleet-wide effects. For highway engines, we made the assumption that all future engines will be equipped with EGR beginning with the 2002 model year. We then estimated the fractional contribution that 2002 and later model year engines are expected to make to the heavy-duty diesel NOx inventory. The results are shown in Table IV.A-3.

Table IV.A-3
Fraction of NOx inventory from EGR-equipped engines

Calender year	Fraction of highway inventory
2002	0.05
2003	0.13
2004	0.22
2005	0.30
2006	0.38
2007	0.45
2008	0.51
2009	0.57
2010	0.63

The remainder of the highway NOx inventory would come from engines that do not have EGR. These fractions can be used to weight the results of the default and technology group L models to derive an estimate for the entire in-use fleet of highway engines.

For nonroad engines, EGR may play a role in meeting future emission standards. However, EGR is unlikely to be used prior to 2006, and in fact manufacturers may choose to use aftertreatment instead. Given EGR's uncertain future in nonroad engines, we have not estimated the contribution that EGR-equipped engines may make to the nonroad inventory. Until such an estimate can be made with greater certainty, we propose that the default NOx model be used to represent all nonroad engines.

B. Application to heavy-duty highway fleet

The Unified Model can be used to evaluate the impacts of changes in diesel fuel on emissions of NOx, PM, and HC for the current fleet of heavy-duty highway diesel vehicles. It cannot be applied to light-duty diesel vehicles because we do not have sufficient information to determine if light-duty vehicles respond in the same way to changes in diesel fuel properties as heavy-duty engines (see further discussion of light-duty in Section VI). We have determined that the Unified Model can be applied to heavy-duty nonroad diesel engines with appropriate caveats and distinctions (see Section IV.E below).

In using the Unified Model, it is the percent change in emissions that is most relevant. The equations as described in Section III.A.3 do permit calculation of emissions in g/bhp-hr, but these emission estimates should not be used as the basis of inventory estimates. Instead, the model equations should be used to calculate the percent change in emissions resulting from a change from one fuel to another. This percent change can then be applied to the inventory estimates for a particular region that have been determined separately according to accepted procedures. Note that for those parties wanting to evaluate the inventory impacts of changes to nonroad diesel fuel, or changes to highway diesel fuel sold in a particular area, it may be necessary to generate an alternative baseline fuel rather than use the nationwide average fuel summarized in Table III.D-1.

The calculation of a percent change in emissions requires that a baseline fuel be established. Under most circumstances the most appropriate baseline fuel would be the national average highway diesel fuel. This baseline is discussed in Section III.C.1, and the model transformation constants in Table III.C.1-2 convert the equations in g/bhp-hr into equations in terms of percent change. The Unified Model can also be used with an alternative baseline if one can be established with sufficient precision.

The predictive capabilities of the Unified Model will be a function of whether the candidate fuel represents a real, in-use fuel. If the model is being used to evaluate a fuel that already exists and whose properties have been measured, or to evaluate a fuel which represents the average of a selection of in-use fuels, this criterion is obviously fulfilled. If the fuel being evaluated with the model is instead conceptual, care must be taken to ensure that the fuel represents something the refiners would or could actually produce.

As discussed in Section IV.A above, we determined that the default models for NOx, PM, and HC should be sufficient for representing the current in-use fleet of heavy-duty highway diesel vehicles. The lack of precise information on the fraction of the fleet represented by specific technology groups and the fact that the inclusion of emission impacts from technology group-specific equations would not substantially affect the predictions for the current fleet led us to this conclusion. However, technology group L is an exception for NOx because EGR-equipped engines are expected to become an increasing fraction of the fleet in the future, and the additized cetane effect for EGR-equipped engines appears to run opposite to that for the rest of the fleet. Therefore, we propose that the emission impacts for changes in diesel fuel properties should be based on both the default and the technology group L models for NOx, and on the default models for PM and HC.

As described in Section IV.A above, we have estimated the contribution that EGR-equipped engines make to the fleet-wide NOx inventory based on the assumption that all 2002 model year and later heavy-duty diesel vehicles will have EGR. This approach provides us with a means of weighting the predicted percent change effects from the default NOx model and the technology group L NOx model. The weighting factors are shown in Table IV.B-1. The constants "a" and "b" appear in the final NOx equation below.

Table IV.B-1
Highway weighting factors for NOx model percent change predictions

Calender year	Default NOx Model Constant "a"	Tech group L NOx model Constant "b"
2002	0.95	0.05
2003	0.87	0.13
2004	0.78	0.22
2005	0.70	0.30
2006	0.62	0.38
2007	0.55	0.45
2008	0.49	0.51
2009	0.43	0.57
2010	0.37	0.63

<u>The final NOx model for highway vehicles is:</u>

$$
\begin{aligned}
\%\text{ change in NOx emissions} = {} & a \times 33.883 \times \exp(- 0.002779 \times \text{cetane difference} \\
& + 0.002922 \times \text{aromatics, vol\%} \\
& + 1.3966 \times \text{specific gravity} \\
& - 0.0004023 \times \text{T50, }^{o}\text{F}) \\
& + b \times 33.776 \times \exp(+ 0.001172 \times \text{cetane difference} \\
& + 0.002922 \times \text{aromatics, vol\%} \\
& + 1.3966 \times \text{specific gravity} \\
& - 0.0004023 \times \text{T50, }^{o}\text{F}) - 100
\end{aligned}
$$

<u>The final PM model for highway vehicles is:</u>

$$
\begin{aligned}
\%\text{ change in PM emissions} = 14.735 \times \exp(& - 0.004521 \times \text{natural cetane} \\
& - 0.04825 \times \text{cetane difference} \\
& + 0.001009 \times \text{natural cetane} \times \text{cetane difference} \\
& + 0.002157 \times \text{aromatics, vol\%} \\
& + 0.00008386 \times \text{sulfur, ppm} \\
& + 2.3708 \times \text{specific gravity} \\
& - 0.07193 \times \text{oxygen, wt\%}) - 100
\end{aligned}
$$

<u>The final HC model for highway vehicles is:</u>

$$
\begin{aligned}
\%\text{ change in HC emissions} = 98035 \times \exp(& - 0.1875 \times \text{natural cetane} \\
& + 0.001571 \times \text{natural cetane}^{2} \\
& - 0.1880 \times \text{cetane difference}
\end{aligned}
$$

$$+ 0.003507 \times \text{natural cetane} \times \text{cetane difference}$$

$$- 0.0009809 \times \text{T10, } {}^{o}\text{F}$$

$$- 0.002448 \times \text{T50, } {}^{o}\text{F} \qquad) - 100$$

Note that these equations must be used in the context of the valid range limits and extrapolations described in Section III.D.

C. Biodiesel

There has been increasing interest in recent years in the use of biodiesel, soy or animal fat-based esters that can be used as a substitute for petroleum-based diesel fuel. Several studies have found HC and PM benefits from the use of biodiesel, and its lubricity characteristics and renewability are also motivators for its use. Several municipalities and States are considering mandating the use of low levels of biodiesel in diesel fuel. Having an estimate of the emission benefits of biodiesel would be a valuable element in any decision to promote or mandate the use of biodiesel.

In reviewing data for inclusion in our database, we found several studies that examined oxygenated fuels, including biodiesel. Many of these studies did not include the detailed fuel property or emissions measurements that would have been necessary for use in our modeling effort. Of those studies that did contain sufficient data for inclusion in our database, only three studies included biodiesel testing. These three studies contributed only three separate biodiesel blends to the database, out of 300 total fuels.

Given the fuel properties that we selected for inclusion in our model, all three biodiesel fuels in our database were missing at least one of those fuel properties. For instance, two of the biodiesel fuels contained all fuel property data except distillation measurements. The third biodiesel included all fuel property data except the oxygen content (we did not make estimates of missing fuel property measurements). As a result, given the approach we took to model development, none of the three biodiesel blends in our database was actually included in the regressions. Thus, our model cannot be used to evaluate the emission effects of biodiesel.

Even if we had chosen an alternative set of fuel properties on which to base our regression in order to include all three biodiesel fuels in the regressions, it may still not have been appropriate to permit use of our model for evaluating biodiesel. Biodiesel can be blended into petroleum-based diesel fuel at any concentration, and it is as yet unclear if the emission effects of such addition would correlate linearly with the biodiesel blend fraction. Since we have only two biodiesel fuels with oxygen measurements in our database, nonlinear effects cannot be captured in our model. We also do not have sufficient information to determine if different types of biodiesel (from different feedstock sources or processing) have different effects on emissions.

Despite that fact that our model cannot be used to evaluate biodiesel blends, having estimates of the emission benefits of biodiesel would be invaluable to anyone considering its use. We have therefore decided to conduct an independent study of biodiesel emission effects. Although this study is unlikely to generate a model of the sort presented in this discussion document, it will include a thorough investigation of currently available data on biodiesel emission effects with the intention of assessing its sufficiency for estimating emission impacts for the current fleet. This study will be conducted over the next few months, with a draft report expected by late in 2001.

D. Other oxygenates

In constructing our database, we included any studies that investigated oxygenated diesel fuels, making no restrictions on the types of oxygenates that would be considered. As a result, a total of 21 oxygenated test fuels were included in our database. However, 15 of these fuels were missing measurements for one or more fuel properties, and so were effectively excluded from our model development. Of the remaining six fuels, only three types of oxygenates were represented, as shown in Table IV.D-1.

Table IV.D-1
Oxygenated fuels arising in regressions

Study	Fuel ID	Oxygenate	Oxygen, wt%
VE-10	D	Monoglyme	2.09
VE-10	E	Monoglyme	3.64
VE-10	F	Diglyme	2.24
VE-10	G	Diglyme	4.02
VE-10	I	Diglyme	4.19
SAE 972898	K	C11 heavy alcohols	0.3

As we conducted our regression analyses, we permitted oxygen terms (in weight percent oxygen) to appear in the model. We determined that there was insufficient data to permit oxygenate-specific terms. Thus the use of our model to represent oxygenated diesel fuels must be conducted on a generic basis with no specific reference to the type of oxygenate.

As the table shows, the types of oxygenates actually represented in the regressions that produced our models are quite limited, in comparison to the broad array of oxygenates available for blending into diesel fuel. As a result we determined that our models should only be used to represent fuels containing the types of oxygenates that actually played a role in the regressions. In addition, the use of unspecific "C11 heavy alcohols" in SAE paper number 972898 is unlikely to have had any appreciable influence on the correlation of oxygen content with emission due to the low concentration of this oxygenate. We do not believe, therefore, that alcohols should be evaluated with our model, either.

The only oxygenates that we believe should be evaluated with our model are glycol ethers similar to monoglyme and diglyme (proper names: ethylene glycol dimethyl ether and diethylene glycol dimethyl ether). The emission impacts of other oxygenated diesel fuels should be evaluated based on data which is specific to the oxygenate in question.

E. Application to CI nonroad fleet

Nonroad compression-ignition engines are an important portion of the diesel fleet and an important contributor to inventories of regulated pollutants. Therefore, in addition to understanding the correlation of diesel fuel parameters with emissions from highway engines, it is important to understand this correlation in nonroad engines.

However, there are very few studies of fuel effects in nonroad engines and it was not possible to develop a separate model for nonroad. For this reason, we considered options for applying the results of the Unified Model for highway vehicles to the nonroad fleet. There are several issues associated with this type of extrapolation, some of which are discussed below and in Section VII.B.6. We welcome comments on the degree to which our model can be applied to nonroad. Note that a new study that does look at fuel effects in nonroad engines will become available soon and offers an opportunity to test our assumptions that our Unified Model can be appropriately applied to nonroad. We will be evaluating this data in the coming months.

Most nonroad engines use technologies similar to those found in highway vehicle engines, although in a given year, the highway vehicle technology is generally more advanced. Thus, subgroups of nonroad engines can be mapped to appropriate subgroups of highway vehicle engines. Furthermore, our Unified Model suggests that most technologies exhibited a similar response to variations in fuel parameters. Thus, in most cases, the distinctions between nonroad and highway vehicle technologies may not be important for the purpose of evaluating relative emission effects of fuel changes. On the basis of technology, then, we believe it is appropriate to apply the Unified Model to nonroad.

There are some concerns that the type of operation that nonroad engines experience may be sufficiently different from the operation of highway vehicles that our Unified Model, based on test cycles designed to represent highway driving, may not be applicable to nonroad. However, there are a variety of test cycles which could represent nonroad applications which are currently being evaluated. The current body of data on nonroad engine cycles is insufficient to indicate whether the effect of changes in diesel fuel properties will affect emissions differently for nonroad engines than for highway engines. On the basis of the information we currently have, then, we believe that the relative effects exhibited by the Unified Model are applicable to nonroad. See the additional discussion of this issue in Section VII.B.6.

As for application to highway engines, we propose that the default models we developed using our Unified Approach be applied to nonroad without accounting for the technology group-specific models that are likely to represent only a small portion of the fleet (see Section IV.A). For highway applications, we made one exception for EGR-equipped engines based on the expectation that EGR will play a more prominent role in the future. However, as discussed in Section IV.A, we do not have the same level of confidence that EGR will play a prominent role in nonroad engines. Therefore, we do not believe it appropriate to introduce weighting factors for technology group L into the final equations when they are used to represent nonroad.

The final NOx model for nonroad engines is:

$$\%\text{ change in NOx emissions} = 33.883 \times \exp\left(\begin{aligned} &- 0.002779 && \times \text{cetane difference}\\ &+ 0.002922 && \times \text{aromatics, vol\%}\\ &+ 1.3966 && \times \text{specific gravity}\\ &- 0.0004023 && \times \text{T50, }^{o}\text{F} \end{aligned}\right) - 100$$

The final PM model for nonroad engines is:

$$\%\text{ change in PM emissions} = 14.735 \times \exp\left(\begin{aligned} &- 0.004521 && \times \text{natural cetane}\\ &- 0.04825 && \times \text{cetane difference}\\ &+ 0.001009 && \times \text{natural cetane} \times \text{cetane difference}\\ &+ 0.002157 && \times \text{aromatics, vol\%}\\ &+ 0.00008386 && \times \text{sulfur, ppm}\\ &+ 2.3708 && \times \text{specific gravity}\\ &- 0.07193 && \times \text{oxygen, wt\%} \end{aligned}\right) - 100$$

The final HC model for nonroad engines is:

$$\%\text{ change in HC emissions} = 98035 \times \exp\left(\begin{aligned} &- 0.1875 && \times \text{natural cetane}\\ &+ 0.001571 && \times \text{natural cetane}^{2}\\ &- 0.1880 && \times \text{cetane difference}\\ &+ 0.003507 && \times \text{natural cetane} \times \text{cetane difference}\\ &- 0.0009809 && \times \text{T10, }^{o}\text{F}\\ &- 0.002448 && \times \text{T50, }^{o}\text{F} \end{aligned}\right) - 100$$

Note that these equations must be used in the context of the valid range limits and extrapolations described in Section III.D.

Section V Diesel Fuel Property Effects On Toxics

A. Introduction

This section considers the impact of diesel fuel properties and qualities on toxics emissions. Toxics emissions can be reduced via control of criteria pollutants such as oxides of nitrogen (NOx), volatile organic compounds (VOCs), carbon monoxide (CO), and particulate matter (PM). For instance, our recently promulgated diesel fuel rule [66 FR 5002, January 18, 2001] limits the maximum sulfur level of on-highway diesel to 15ppm. This enables the use of aftertreatment technology for the control of PM and NOx emissions (e.g., traps and NOx adsorbers). As a result, certain types of toxics emissions are also expected to be reduced. However, our focus here is to predict the change in toxics emissions solely through specific fuel quality changes.

EPA's Mobile Source Air Toxics (MSAT) list specifies 21 compounds emitted from motor vehicles that are known or suspected to cause cancer or other serious health effects. The list includes VOCs, metals, diesel particulate (DPM) and diesel exhaust organic gases (DEOG). The specific compounds are shown in Table V.A.1. The selection process for including, adding and removing compounds from the list is described in the recently promulgated rule, "Control of Emissions of Hazardous Air Pollutants from Mobile Sources" [66 FR 17230, March 29, 2001]. While that rule focused on toxic compounds emitted from gasoline-fueled vehicles, many of the same compounds are found in diesel exhaust organic gases. In that rule, the toxics regulated (as a group) are benzene, 1,3-butadiene, formaldehyde, acetaldehyde and polycyclic organic matter (POM).

Table V.A-1
List of Mobile Source Air Toxics (MSAT)

1. Acetaldehyde	8. Dioxin/Furans	15. MTBE
2. Acrolein	9. Ethylbenzene	16. Naphthalene
3. Arsenic Compounds	10. Formaldehyde	17. Nickel Compounds
4. Benzene	11. n-Hexane	18. POM
5. 1,3 - Butadiene	12. Lead Compounds	19. Styrene
6. Chromium Compounds	13. Manganese Compounds	20. Toluene
7. Diesel Particulate Matter + Diesel Exhaust Organic Gases (DPM + DEOG)	14. Mercury Compounds	21. Xylene

As will be seen in the results of the studies reviewed here, many of these compounds are also found in diesel emissions.

Few studies of the effects of diesel fuel quality on toxics emissions exist. Most studies which evaluate diesel fuel quality changes have only measured their impact on criteria pollutants. Only a few studies report emissions of carbonyls (aldehydes and ketones) or/and gas phase toxic hydrocarbons such as benzene and 1,3-butadiene. Still, the limited information available can be useful for directionally indicating the likely outcome of a diesel fuel quality change on toxics., and also for directing researchers to future work in this area. Three studies which evaluated diesel fuel quality changes and also reported emissions of certain toxic compounds are discussed below.

B. Studies Which Measured Emissions of Toxics

Of the studies which were included in the development of the NOx, PM, and HC models above, only three measured toxic emissions. One was a comprehensive analysis performed for the California Air Resources Board (CARB). The other two studies were performed by Arco Chemical Company and focused on the impact of cetane additives on emissions. These studies are described below, along with a summary of their findings.

The European Programmes on Emissions, Fuels and Engine Technologies (EPEFE) - Light Duty Diesel Study (SAE 961073) also measured certain toxics emissions, and the results are discussed briefly. However, because the speciation measurements were made only for a single test of each fuel/vehicle combination, they concluded that “a statistical analysis...was not feasible.”

1. CARB Report[13]

The study performed for CARB tested three diesel fuels in a Cummins L10 engine. The three fuels included a pre-1993 diesel fuel (beginning in 1993, CARB regulations limited diesel sulfur to 5 ppm, minimum cetane index of 40 and maximum aromatic content to 10 vol%), a low aromatic fuel, and an alternative formulation which should achieve the same emissions reductions as the low aromatic fuel. The fuel specification ranges are shown in Table V.B.1-1.

Table V.B.1-1
Diesel Fuel Specification Ranges

	Pre-1993	Low Aromatic	Reformulated
Aromatics (vol%)	33	10 max	20-25
Sulfur (ppm)	<5000	500 max	100-300
Cetane number	>40	48 min	50-55
PAH (wt%)	8	1.4 max	2-5
Nitrogen (ppm)	300-600	10 max	40-500

API gravity measurements of the fuels were 32.8, 37.2 and 37.1, respectively.

Total hydrocarbon, NOx and PM emissions were all reduced for both the low aromatic fuel and the reformulated fuel compared to the Pre-1993 fuel (Table V.B.1-2). However, only the total hydrocarbon and PM emissions changes from the Pre-1993 fuel were deemed statistically significant[j].

Table V.B.1-2

	Mean Weighted Total Emissions[k]					
	NOx		THC		PM	
	gm/bhp-hr	%[l]	gm/bhp-hr	%	gm/bhp-hr	%
Pre-1993	4.77	---	0.53	---	0.224	---
Low Aromatic	4.44	-7.1	0.47	-11	0.183	-18
Reformulated	4.64	-2.7	0.5	-5.7	0.186	-17

Though carbonyls increased in all cases compared to the Pre-1993 fuel (Table V.B.1-3), only the acetaldehyde results for both the low aromatic and reformulated fuels, and the acrolein results for the low aromatic fuel were deemed statistically significant.

Table V.B.1-3
Carbonyls

	Mean Weighted Total Emissions							
	Formaldehyde		Acetaldehyde		Acrolein		Propionaldehyde	
	mg/bhp-hr	%	mg/bhp-hr	%	mg/bhp-hr	%	mg/bhp-hr	%
Pre-1993	57.12	---	18.15	---	2.14	---	3.69	---
Low Aromatic	58.75	2.8	19.1	5.2	5.79	171	3.92	6.2
Reformulated	59.83	4.7	19.93	9.8	2.42	14	4.13	12

The direction of the changes in gas phase emissions of specific hydrocarbons were mixed. The low aromatic fuel showed significant increases (in terms of percent change) for benzene, 1,3-butadiene, toluene and styrene emissions. This fuel also significantly reduced ethylbenzene, o-xylene and m&p-xylene (Tables V.B.1-4A, B, C). The results of the low aromatic fuel were statistically significant only for benzene, toluene, and m&p-xylene. There were no statistically significant differences between the Pre-1993 and reformulated fuel gas phase hydrocarbon emissions.

---

[j] Significant at 95% confidence limit using Fisher's Protected Least Significant Difference Test.

[k] Weighting of cold start and hot start emissions, 1/7 and 6/7, respectively.

[l] Percent change from the Pre-1993 fuel.

Table V.B.1-4A
Gas Phase Hydrocarbons - A

	Mean Weighted Total Emissions			
	Benzene		1,3-Butadiene	
	mg/bhp-hr	%	mg/bhp-hr	%
Pre-1993	5.9	---	1.8	---
Low Aromatic	8.03	36	2.46	37
Reformulated	5.81	-1.5	1.84	2.9

Table V.B.1-4B
Gas Phase Hydrocarbons - B

	Mean Weighted Total Emissions							
	Toluene		Ethylbenzene		O-Xylene		m&p-Xylene	
	mg/bhp-hr	%	mg/bhp-hr	%	mg/bhp-hr	%	mg/bhp-hr	%
Pre-1993	1.93	---	1.22	---	0.78	---	2.09	---
Low Aromatic	2.26	17	0.67	-45	0.61	-21	1.24	-40
Reformulated	1.86	-3.6	1.18	-3.6	0.88	12	2.14	2.5

Table V.B.1-4C
Gas Phase Hydrocarbons - C

	Mean Weighted Total Emissions			
	Styrene		Naphthalene	
	mg/bhp-hr	%	mg/bhp-hr	%
Pre-1993	1.27	—	1.69	---
Low Aromatic	1.58	24	1.74	2.9
Reformulated	1.45	14	1.27	-24

An overall decrease was seen in particle-bound Polycyclic Aromatic Hydrocarbon (PAH) emissions based on hot start sampling only. Nitro-PAH hot-start emissions changes compared to emissions from the Pre-1993 fuel were mixed directionally. For specific compounds, the percent change in emissions from the Pre-1993 fuel ranged from -54% to +35% for the low aromatic fuel and -39% to +27% for the reformulated fuel. In half the cases, due to analytical limits, no changes were noted between the Pre-1993 fuel and the other two fuels. Results of single hot start sampling showed reductions in vapor phase PAH emissions; the reductions for the low aromatic fuel were particularly large, for several compounds over 85%.

2. Arco Chemical Company Cetane Improvement Additive Studies

In two related studies, Arco Chemical Company compared the emissions of a base fuel with the emissions of a fuel which contained either a peroxide-based cetane improvement additive or a conventional cetane improvement additive, 2-ethylhexyl nitrate. The minimum cetane number increase was nine, and the emission measurements were based on hot-start cycles only. The first study[14] looked at a single base fuel (compared to additized fuels); the second study[15] looked at three different levels of each additive. A single engine, Detroit Diesel Corp., 1991 Prototype Series 60, was used for all tests.

For a given base fuel, the additized fuels produced similar hydrocarbon reductions. These reductions ranged from 40-75%. Speciated toxics emissions, including benzene, 1,3-butadiene, aldehydes and ketones, were also significantly reduced with the cetane-improved fuels compared to the corresponding base fuels. A summary of the toxics emission results is shown in Table V.B.2-1. The percent reductions from the corresponding base fuel emissions are shown in Table V.B.2-2. These reductions are in line with the reductions in hydrocarbon emissions. .

Table V.B.2-1
Emission Results for Additized Fuels

	0.40% ethylhexyl nitrate	0.55% ethylhexyl nitrate	0.65% ethylhexyl nitrate	0.70% ethylhexyl nitrate	0.50% peroxide	0.70% peroxide	0.75% peroxide	0.80% peroxide
Cetane number	56	52	49	57	57	53	49	58
Emissions (mg/bhp-hr)								
Acetaldehyde	11	9	18	12	14	10	14	15
Acetone	11	3.7	7	4	18	5.8	7	4
Acrolein	3	3	5	2	3	3	4	3
Benzaldehyde	1	0.9	0.5	0	2	0.7	1.0	1
Benzene	0.8	---	1.6	1.7	1.4	---	0.8	1.0
1,3-Butadiene	1.7	---	2	1.4	1.4	---	1.8	1.1
Crotonaldehyde	3	1.2	5	2	4	1.0	4	1
Formaldehyde	25	23	47	25	26	24	38	32
Hexanaldehyde	2	0.7	8	2	2	0.6	6	1
Isobutyraldehyde + MEK	1	1.2	2	0.4	2	1.0	2	2
Propionaldehyde	3	2	9	3	4	1	7	4

Table V.B.2-2
Changes from Base Fuel

	0.40% ethylhexyl nitrate	0.55% ethylhexyl nitrate	0.65% ethylhexyl nitrate	0.70% ethylhexyl nitrate	0.50% peroxide	0.70% peroxide	0.75% peroxide	0.80% peroxide
Cetane number (absolute change)	+10	+9	+10	+15	+11	+10	+10	+16
% Change in Emissions								
Acetaldehyde	-70	-62	-66	-68	-62	-58	-74	-60
Acetone	-68	-63	-63	-69	-47	-42	-63	-69
Acrolein	-70	-57	-50	-78	-70	-57	-60	-67
Benzaldehyde	-67	-55	-92	-100	-33	-65	-83	-67
Benzene	-62	----	-73	-39	-33	---	-86	-64
1,3-Butadiene	-29	----	-66	-61	-41	---	-69	-69
Crotonaldehyde	-57	-57	-75	-83	-43	-64	-80	-92
Formaldehyde	-44	-62	-70	-67	-42	-60	-75	-58
Hexanaldehyde	-71	-82	-80	-50	-71	-84	-85	-75
Isobutyraldehyde + MEK	-83	-74	-80	-90	-67	-79	-80	-50
Propionaldehyde	-73	-71	-83	-70	-64	-86	-87	-60

3. EPEFE Light Duty Diesel Study

As mentioned above, the toxics measurements described in the light-duty study conducted by the European Programme on Emissions, Fuels and Engine Technologies (EPEFE)[16] were not sufficient to allow statistical analysis. Nonetheless, the summary of their findings is informative and would provide a helpful start when comparing results of other test programs or looking for starting points for future test programs.

Table V.B.3-1
EPEFE Toxics Summary

Parameter	Effect on emissions
Engine technology vs. Fuel quality	"...engine technology has a greater effect on air toxic emissions than changes in fuel quality."
Density and polyaromatics	a. Decreasing density decreased benzene and 1,3 - butadiene in line with THC b. Decreasing polyaromatics increased benzene c. Decreasing density and polyaromatics decreased formaldehyde d. Decreasing density (at low polyaromatics) or decreasing polyaromatics (at low density) decreased acetaldehyde
Cetane number	a. Increasing cetane number decreased benzene and 1,3 - butadiene in line with THC b. Increasing cetane number decreased acetaldehyde
Back end distillation (T95)	a. Decreasing T95 may increase benzene b. Decreasing T95 increased formaldehyde

C. Conclusions and Next Steps

The results of the studies evaluated for this staff discussion document show that changes in certain diesel fuel qualities, such as cetane number, may significantly affect toxic emissions from diesel engines. For other diesel fuel qualities, such as sulfur or aromatic content, the results are mixed (a given change in fuel quality increases one type of emission while decreasing another) or are not statistically significant. Clearly more testing of diesel fuels of varied composition is needed. Such testing should further address which fuel properties are most important for controlling individual toxic compounds, and whether conclusions can be drawn for specific fuel formulations rather than individual fuel properties.

Section VI Diesel Fuel Effects In Light-Duty Vehicles

A. Introduction

The available data on fuel effects in light-duty diesels are quite limited. As a result, it was not possible to develop a model for light-duty vehicles. Instead, we reviewed the data for consistent trends in fuel effects. The studies[17,18,19,20,21] examined the effects of diesel fuel properties on exhaust emissions (i.e., PM, NOx, HC, and CO) for light-duty vehicles/engines. The researchers focused mainly on four key properties in their investigations of diesel fuel effects: density, aromatics content, cetane number, and distillation range. Even though the effect of sulfur on diesel particulate formation is well established, some investigators also examined how sulfur interacted with oxidation catalysts and various test cycles to affect PM formation (See references 18, 20, 21).

The studies tested light-duty vehicles or trucks made in the 1990s. These vehicles/engines encompassed a combination of the following technologies:

- Electronically or mechanically controlled fuel injection system
- Naturally aspirated (NA) or turbocharged (TC) engines, some with intercooling
- Direct injection (DI) or pre or swirl chambers indirect injection (IDI) combustion chambers
- Exhaust Gas Recirculation (EGR) - electronically and mechanically controlled
- Oxidation Catalysts

The test cycles used in the light-duty studies included the European MVEG test cycles (ECE15+EUDC), the European ECE R49, and the U.S. FTP. For the purpose of our light-duty analysis, we focused mainly on vehicle testing results, although comparisons were also made with some results obtained from engine testing. Table VI.A-1 lists the ranges of diesel fuel properties examined across various studies.

Table VI.A-1
Ranges of Fuel Properties Examined

Property	density (kg/m^3)	poly-aromatics (wt%)	cetane number	T95 (°C)	viscosity cSt @40°C
Range	805-857	0-11	45-70	248-391	1.3-3.9

B. Individual Studies

1. EPEFE Study

During the mid-1990s, an initiative was carried out by the European Automobile and Oil Industries - the European Programme on Emissions, Fuels and Engine Technology (EPEFE). This program examined a fleet of 19 vehicles (17 passenger cars, 2 light duty trucks), all fitted with oxidation catalysts. All testing were done against the MVEG test cycle (ECE15+EUDC). The objective of this program was to focus on density, poly-aromatics, cetane number, and T95. The investigators studied the poly-aromatics content but did not report the total aromatics content. They examined how these fuel variables affected PM, NOx, HC, and CO emissions. Table VI.B.1-1 shows the eleven fuels in the fuel matrix. The fuels were designed to decorrelate the individual effects of density, poly-aromatics content, cetane number, T95, and especially density and poly-aromatics content which are closely intercorrelated in market fuels.

Table VI.B.1-1
EPEFE Fuel Properties

Fuel No.	Density kg/m^3	Poly-aromatics %	Cetane Number	T95 Celsius
EPD1	829.2	1.0	51.0	344
EPD2	828.8	7.7	50.2	349
EPD3	857.0	1.1	50.0	348
EPD4	855.1	7.4	50.3	344
EPD5	828.8	7.1	50.6	346
EPD6	855.5	7.6	50.2	371
EPD7	826.9	1	49.5	326
EPD8	855.1	7.3	54.8	345
EPD9	855.4	8	59.1	344
EPD10	826.6	1.1	58.0	347
EPD11	827	0.9	57.1	329

The investigators performed extensive data analysis that included pairwise comparisons, submatrix analysis, and full regression analysis. Specifically, they separated the fuel matrix into three individual subsets of fuels, allowing comparisons of fuels by varying in one specified property only:

Matrix (1): EPD1-5 to investigate the effect of density and poly-aromatics
Matrix (2): EPD1,7,10,11 at low density and EPD 4,8,9 at high density to investigate the effects of cetane number

Matrix (3): EPD 1,7,10,11 at low density and EPD 4,6 at high density to investigate the effects of T95

2. Lange Study

Lange et al.[18] tested a Mercedes-Benz 250 D (2.5 liter) engine typical of the 1991-1993 model years. This passenger vehicle had a 5 cylinder naturally aspirated IDI engine, and it was equipped with an EGR and an oxidation catalyst, enabling it to meet 91/441/EEC emissions standards. The researchers reported the effect of fuel changes on PM and NOx emissions. They designed three sets of diesel fuels (12 fuels total) for vehicle emission testing over the ECE15+EUDC cycle. The fuel properties and chemical composition are shown in Table VI.B.2-1.

Table VI.B.2-1
Fuel Properties and Chemical Composition

	Unit	SET 1					SET 2				SET 3		
Fuels		1	2	3	4	5	6	7	8	9	10	11	12
Density	g/ml	0.826	0.826	0.826	0.826	0.826	0.837	0.807	0.814	0.834	0.844	0.838	0.842
Distillation													
T10E	ºC	228	228	227	229	228	219	234	213	235	224	220	223
T50E	ºC	278	272	272	281	270	269	296	231	288	280	279	281
T90E	ºC	323	324	325	326	326	326	346	269	345	339	350	344
T95E	ºC	335	335	337	338	338	348	355	279	368	358	371	364
FBP	ºC	347	350	351	353	354	368	364	293	380	381	389	389
Cetane no.		56.4	56.4	56.5	56.4	56.1	50.0	70	54	59	48	51	50
Viscosity @ 40ºC	mm^2/s	3.12	3.09	3.08	2.90	2.88	2.82	3.90	1.93	3.85	3.11	3.26	3.35
Sulfur content	ppm m	<10	220	450	960	1800	500	<10	10	45	680	450	430
Aromatics													
Mono	m%	7.95	9.74	11.61	16.57	16.72	24.9	<0.05	9.7	4.1	23.4	22.4	22.4
DI	m%	0.05	0.20	0.56	2.04	2.09	1.9	<0.05	0.1	0.1	2.7	1.7	1.7
TRI+	m%	0.02	0.46	0.73	1.21	1.04	1.4	<0.05	<0.05	<0.05	3.0	1.3	1.3
Poly	m%	0.07	0.66	1.29	3.25	3.13	3.3	<0.05	0.1	<0.1	5.7	3.0	3.0
Total	m%	8.02	10.39	12.90	19.82	19.84	28.3	<0.05	9.8	4.2	29.1	25.4	25.4

The three sets of fuels were designed for studying the effect of sulfur, mono- and poly-aromatics content, density, cetane number, and distillation properties on PM and NOx emissions. The objectives for individual sets of fuels are described in the following:

Set (1): Fuels 1-5 were designed to decorrelate fuel sulfur content from other properties.

Set (2): Fuels 6-9 were to decorrelate fuel density from aromatics (i.e., fuel pairs 6 and 9 or 7 and 8 were similar in density, but significantly different total aromatics content.) No attempt was made to control the variation in cetane number and distillation in this fuel set.
Set (3): Fuels 10-12 focused on the poly-aromatics/distillation properties.

The authors studied fuel effects by making pairwise comparisons as well as regression analyses across all 12 fuels in order to identify important fuel properties. However, the fuels were not designed for such a pooled analysis across the three sets and, therefore, significant intercorrelations existed when the individual fuel sets were pooled together.

3. Bertoli Study

In another study, Bertoli et al.[19] studied a matrix of 14 fuels on a passenger vehicle that met the ECE 15:04 regulations. In this study, they tested a turbocharged, direct injection 2.5 liter displacement engine over a cycle representative of the ECE 15 cycle. They measured PM, NOx, HC, and CO emissions. Table VI.B.3-1 lists the fuel properties examined.

Table VI.B.3-1
Fuel Properties

Fuel	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Density [g/ml]	0.829	0.836	0.806	0.827	0.820	0.811	0.821	0.829	0.827	0.841	0.814	0.817	0.814	0.818
Sulfur [ppm]	1300	9420	50	445	2	1	542	1050	1200	2320	2	1	1	1
Distill. [ºC]														
10%	200	221	179	217	214	211	212	213	210	210	213	213	208	206
50%	274	283	242	279	272	268	265	269	256	254	260	261	252	245
95%	387	391	381	386	382	380	380	380	378	385	349	352	348	347
Cetane number	57.1	54	52.7	57	59	62.3	56.8	57.4	52.6	47	61	60.1	58.7	56
Aromatics [m%]														
mono-	10.7	14.54	5.67	18.10	14.80	6.1	4.1	4.1	7.8	9.8	5.1	4.9	4.2	3.9
di-	5.5	6.6	1.04	5.60	2.00	0.5	2.4	6.6	6.9	10.7	1	0.1	0.4	0.2
tri-	0.7	1.0	0	0.50	0.10	0	1.0	3.0	0.1	0.1	0	0	0	0
total	16.9	22.1	6.7	24.2	16.90	6.6	7.5	13.7	14.8	20.6	6.1	5.0	4.6	4.1
S-arom	0.9	5.0	0.3	0.3	0	0	0.3	0.7	1.3	1.4	0	0	0	0

They analyzed the correlation matrix of the fuel variables and found a strong correlation between density and the sum of di- and tri-aromatics content. The researchers decided to treat them as a single variable and regressed on Σ di-tri-aromatic compounds in their analysis. In addition, the investigators focused on the cetane number, sulfur, T95, and total aromatics content. They carried out a linear regression analysis with these parameters as independent variables and emissions as the dependent variables.

C. Results and Discussion

All three studies found that an increase in either the poly- (or Σ di- and tri-) aromatics content or density resulted in higher PM emissions. However, variations in other fuel properties led to inconsistent changes in emissions. Factors such as engine design or vehicle technologies, engine operating conditions, and the test cycle all played important interactive roles with fuel properties in influencing pollutant emissions. Due to a scarcity of available data, it was not possible to separate all these variables in order to isolate the fuel effects on emissions. Nevertheless, some additional conclusions could be drawn regarding fuel effects on pollutant emissions. A summary of the magnitude and/or directional changes of emissions from varying fuel properties in each study is given in this section.

1. EPEFE Study

Results from the EPEFE study[17] indicated that while individual vehicles responded to variations in certain fuel properties consistently, different vehicles showed significantly different responses to changes in other fuel properties, both in magnitude and direction. Upon averaging the emission results across all 15 vehicle models, the EPEFE researchers observed the emission changes summarized in Table VI.C.1-1.

Table VI.C.1-1
EPEFE Averaged Percentage Changes in Emission over Combined ECE15+EUDC Cycles

Emission effects due to increasing parameters indicated:	PM	NOx	HC	CO
density: 827 to 855 kg/m^3	+19%	-2%	+18%	+17%
poly-aromatics: 1 to 8 %m/m	+5%	+3%	-5.5%	-4%
cetane: 50 to 58	+5%	+1%	-26%	-25%
T95: 325 to 370°C	+7%	-5%	-3%	+2%

The investigators noted that the magnitude of the density effect on NOx emissions was highly dependent on the engine design. We discuss engine technologies interactions with fuel effects in Section VI.D.

The EPEFE study also examined the amount of sulfate formed over the fleet of light duty vehicles, all equipped with oxidation catalysts. Although the fuels explored in this study were not designed to vary the sulfur level, the investigators found differences ranging from 5-10% in sulfate formation for the individual vehicle tested. They noted that the vehicle with the highest sulfate formation was one of the light-duty trucks. The investigators suggested that the high sulfate formation rate in the truck was probably due to its heavier weight compared to a passenger car and the resulting higher engine loads in the EUDC (extra-urban driving cycle) which resulted in higher temperatures, and thus more sulfate production over the catalyst.

2. Lange Study

Lange et al.[18] focused primarily on fuel effects on NOx and PM emissions. They found no fuel effects with respect to NOx emissions. For PM emissions only, the investigators made pairwise comparisons over fuel properties. They found that the mono-aromatics content, cetane number, and distillation did not affect PM emissions. They also concluded that total aromatics were little use in describing fuel effects on emissions, whereas the sulfur content, density, and poly-aromatics content affected PM emissions. Table VI.C.2-1 lists the trends observed in pairwise comparisons.

Table VI.C.2-1
Fuel Effects on PM Emissions over ECE+EUDC Cycles (Lange et al.)

Fuel effects due to increasing parameters indicated:	PM Emissions (g/km); before	PM emissions (g/km); after	Percentage Change
density [a]: 814 to 834 kg/m^3	0.06	0.07	+15%
poly-aromatics: 3.3 to 5.7 %m/m	0.085	0.10	+15%
cetane [b]: 54 to 70	0.06	0.06	0
T90: 269 to 350°C	NC	NC	N/A
sulfur level: 960 to 1800 ppm	0.085	0.1	+15%

a: 814 kg/m^3 (9.7 mass% mono-aromatics) to 834 kg/m^3 (4.1 mass% mono-aromatics)
b: 54 (10 mass% mono-aromatics) to 70 (negligible mono-aromatics)
NC: no correlations found
N/A: not applicable

As shown in Table VI.C.2-1, the results from changing density and cetane indicated that the mono-aromatics content did not affect particulate emissions. This was based on the collective findings that a reduction of mono-aromatics content by 5-6 mass% did not reduce PM emissions, while an increase of mono-aromatics content by 10 mass% did not affect particulate emissions although there was a substantial difference in the cetane number.

With regard to effects due to sulfur level on PM emissions, Lange et al. designed fuels with a diesel sulfur level ranging from <10 to1800 ppm. Apart from the sulfur quantity in fuels, they observed that PM emissions are highly dependent on the driving conditions. They found the level of dependence increases significantly from the least severe cycle to the high speed steady-state cycle when the sulfur level is above 500 ppm: FTP75 < ECE+EUDC < 120 km/h constant speed. Moreover, when they tested the Mercedes over ECE R49 on a diesel fuel containing about 10 ppm sulfur, they noticed that the amount of sulfate produced was greater than that seen at the engine-out level using 450 ppm sulfur fuel. Although the oxidation catalyst was able to reduce the soluble organic fraction of particulate matter, the overall PM emissions at engine-out (using 450 ppm sulfur) and post-catalyst (using 10 ppm sulfur) were similar due to trade off of increased sulfate formation over the vehicle equipped with the oxidation catalyst.

3. Bertoli Study

Bertoli et al.[19] found similar trends as those observed by Lange et al. in that density and di-tri aromatics correlated well with PM emissions. As mentioned previously, density and di-tri aromatics were closely intercorrelated. Their results also showed that the sum of two and three-ring aromatics was far better correlated to PM emissions than the total aromatics content. Furthermore, unlike EPEFE, they found no correlations between T95 and emissions of any pollutant among the fuels they examined. They also found that a reduction of cetane number resulted in increased emissions of NOx, HC, and CO. Because the authors did not provide numerical results as those studies presented in Sections VI.C.1 and VI.C.2, we summarize the trends obtained from their correlation analysis in Table VI.C.3-1.

Table VI.C.3-1
Correlation Trends Observed by Bertoli et al. (ref.)

Fuel Properties	PM	NOx	HC	CO
Σ di- and tri-aromatics ↑	+	NR	NR	NR
cetane number ↓	NC	+	+	+
T95	NC	NC	NC	NC

NC: no correlations found
NR: not reported

4. Summary of Studies

All three studies presented in the previous section found a consistent correlation between increasing fuel density and PM emissions. A similar correlation was found between poly- (or the sum of two and three-ring) aromatics content and PM emissions. However, there were variations among the observations of fuel effects on NOx emissions. Table VI.C.4-1 summarizes various correlations found by these investigators on PM and NOx emissions.

Table VI.C.4-1
Fuel Effects on PM and NOx Emissions

	PM Emissions			NOx Emissions		
Fuel properties	EPEFE[a]	Lange et al.(ref.)	Bertoli et al. (ref)	EPEFE[a]	Lange et al.(ref.)	Bertoli et al. (ref)
density ↑	+	+	+	-[b,c]	NC	NR
cetane number ↑	+	NC	NR	NC[b]	NC	-
Σ di-tri, or poly-aromatics ↑	+	+	+	+	NC	NR
distillation temperature ↑	+	NC	NC	-	NC	NC

NC: no correlations found
NR: not reported
a: fleet averaged results
b: individual vehicle responses varied widely with engine technologies
c: very slight averaged reduction

While the effect due to fuel density on PM emissions has been consistent across various findings, the magnitude of the density effect on PM emissions is related to the engine design and technologies[22,20]. The impact of cetane number on NOx emissions also appears to depend on engine technology. Further discussions on the interactions between fuel properties and engine technologies are provided in Section VI.D.

There is very limited data set on fuel effects on HC and CO emissions. Table VI.C.4-2 summarizes these experimental findings. The two research groups that reported fuel effects on HC and CO emissions agreed that an increase in the cetane number resulted in a reduction of both HC and CO emissions. However, Bertoli found no correlations between the distillation temperature and HC or CO emissions, while correlations were obtained in the EPEFE study.

Table VI.C.4-2
Fuel Effects on HC and CO Emissions

	HC Emissions		CO Emissions	
Fuel properties	EPEFE[a]	Bertoli et al. (ref)	EPEFE[a]	Bertoli et al. (ref)
density ↑	+	NR	+	NR
cetane number ↑	-	-	-	-
Σ di-tri, or poly-aromatics ↑	-	NR	-	NR
distillation temperature ↑	-	NC	+	NC

NC: no correlations found
NR: not reported
a: fleet averaged results

D. Effects of Vehicle Technology and Operation

As mentioned previously, results from various research groups demonstrated that the magnitude of any diesel fuel property alone was generally not a good indicator for projecting the amount of pollutant emissions. This was especially true for determining NOx emissions. The results showed that diesel fuel properties, engine technologies, and driving cycle all played interactive roles in determining the amount of pollutants emitted.

1. DI and IDI Engines

In the EPEFE study[17], an increase in density resulted in a slight reduction of fleet averaged NOx emissions, shown in Table VI.C.1-1. However, individual vehicle responses to density increase were not consistent directionally, even though this group of light-duty vehicles was tested under the same protocol and fuels. They also varied considerably in magnitude. When the density was reduced, emissions data from individual vehicle showed that the half of the fleet with electronic injection responded with increased NOx emissions, while the opposite effect was seen with the remaining half of the fleet. This varying behavior from the light-duty fleet was also seen with NOx emissions when the cetane number of the fuel was varied. As the cetane number was increased, the NOx emissions reduced for DI (mostly electronically controlled) fleet, while the NOx emissions increased for the IDI (mostly mechanically controlled) fleet. The investigators reported that DI vehicles were primarily tuned to control NOx with resulting trade off of the other emissions (e.g., PM, HC, and CO). Consequently, vehicles with electronically controlled injection generally showed higher levels of PM, HC, and CO emissions than mechanically controlled vehicles. Because the engine technologies played such an integral part in how fuel properties would affect emissions, the fuel property should not be taken alone in determining its impact on the pollutant emission levels.

Although the magnitude changes due to fuel effects were generally of the same order between the DI and IDI fleets in the EPEFE study, the DI and IDI fleets displayed a very different sensitivity in cetane number effects on PM emissions. The investigators observed that from PM emissions DI vehicles were about four times more sensitive than those from IDI vehicles, percentage wise. Therefore, their study indicated that under certain circumstances, vehicle technology changes may play an even more significant role than fuel property changes in affecting the amount of pollutant emissions.

2. Sensitivity of Vehicle Response to Engine Parameters

This chapter has thus far focused on fuel parameter studies with little discussions on engine effects such as changes to engine calibration or operating conditions. However, two studies that focus on these effects offer important insights for interpreting the previously discussed studies.

a. Engine Operating Conditions

Beatrice et al carried out an engine study over a 2 liter, turbocharged, DI engine equipped with an EGR system[23]. The fuel matrix examined consisted of 12 different fuels. Focusing on the engine sensitivity to fuel quality in their steady-state testing at various operating (e.g., load, speed, and ambient temperature) conditions, they indicated that the engine sensitivity to fuel quality changes was very different depending on both the operating conditions and the individual pollutant emission under examination. They noticed the sensitivity to fuel quality changes increased at low load and speed, especially for HC emissions. With respect to PM emissions, all test conditions were found to be relevant, while particularly higher sensitivity was noted at retarded timings and during cold operation. However, this was not true for NOx whose behavior was quite flat over varying test conditions. Their study stressed the importance of the interplay between the engine operating conditions and fuel properties on pollutant emissions.

b. Engine Calibration Systems

Another study by Mann et al. focused on how fuel properties influenced the engine management system, thus affecting pollutant emissions[22]. Mann et al. examined the effect of diesel fuels on an electronically controlled, 2 liter DI passenger car engine, equipped with an EGR. Both the injection timing and EGR were controlled by closed-loop strategies. This engine was tested under the European 14 mode test conditions. Mann et al. studied the interplay between the fuel properties and various engine control systems. Specifically, when the density was increased, they noted an increased EGR rate and an advanced injection timing. Advancing injection timing was for controlling PM (trade off for NOx), while the EGR was for controlling NOx emissions (trade off for PM), and these strategies would contribute to competing effects in emission reduction. With this particular engine, the EGR rate dominated, thus resulting in lower NOx emissions. This study demonstrated how the fuel property had led to changes in engine operation settings of competing consequences. Table VI.D.2.b-1 compares the PM and NOx emissions obtained before and after engine calibration modifications due to fuel density change.

Table VI.D.2.b-1
Effect of Engine Calibration Changes on Emissions

Engine Calibration	Fuel density (kg/m^3)	PM emissions (g/km)	NOx emissions (g/km)
Before	829	0.075	0.76
After	857	0.084	0.69

This study clearly illustrated the complex relationships between various engine management components that could impact pollutant emissions. Even though advanced injection timing should lead to higher NOx emissions, the net effect due to an increase in fuel density was NOx reduction by the co-existence of the more dominant EGR effect. Thus, all aspects of the engine systems need to be taken together to assess fuel effects on emissions.

E. Conclusions

We noted a consistent trend across several studies that showed an increase in either density or the poly- (or Σ di- and tri-) aromatics content results in higher PM emissions. Investigators who also examined effects due to both mono- and poly-aromatics content found no correlations between the mono-aromatics content and PM emissions. For other fuel properties, the results indicated a wide variation in diesel fuel effects on NOx emissions. Some investigators found a correlation between cetane number and NOx emissions, while other research groups found no significant fuel effects for NOx emissions over a wide variation in fuel composition. In addition to fuel effects on PM and NOx emissions, several investigators observed that an increase in the cetane number resulted in a reduction of both HC and CO emissions.

The studies also showed that engines with different technologies would respond differently to changes in fuel properties. The varied engine responses may have partly attributed to inconsistencies among various findings in fuel effects on pollutant emissions. The EPEFE study demonstrated that fuel properties such as density or cetane number on the extent of NOx emissions clearly depended on the engine design: DI engine fleets (mostly electronically controlled) had responded in the opposite direction compared to the IDI (mostly mechanically controlled) engines. The investigators also presented results indicating that the amount of pollutant emissions would, in some instances, strongly depend on the engine technologies on the vehicle.

Unlike our results for heavy-duty vehicles, these results collectively suggest the difficulty of projecting changes in light-duty vehicle emissions as a function of diesel fuel parameters. Nevertheless, there is clearly some PM benefit associated with reducing density/poly-aromatics, and HC and CO benefit with an increase in the cetane number. However, the magnitude of emissions reduction is highly uncertain without a full understanding of the specific vehicle design and configurations, and such assessment would require further analysis. Diesel fuel properties, along with existing engine design or vehicle technologies, operating conditions (load, speed, ambient conditions) as well as the driving cycles all play interactive roles in influencing the amount of pollutant emissions.

Section VII What Additional Issues Should Be Addressed?

To assure that our analysis represents the best technical analysis possible at this time, we are making this staff discussion document available in for review and comment. The comment period continues through September, 2001. At the end of the comment period, we will consider the comments received and we will revise our discussion document and our analysis to take those comments into account. We will then finalize a report and make it publically available as an EPA technical report.

Eventually, we plan to incorporate the results of this analysis into EPA modeling tools such as the MOBILE and NONROAD models or their successor models. This will allow emission modelers to better apply the results of this analysis to their inventory estimates and to estimate emissions for a variety of "what-if" scenarios.

In addition to the work EPA plans in finishing this analysis, there are a number of areas that could benefit from further study. While we believe the analysis in our discussion document is sufficient for estimating the emission impacts of changes to diesel fuel within the ranges described in Section III, there are a number of areas that we think could particularly benefit from more test data and analysis. This section summarizes those issues we believe are of the highest importance. We welcome comments on these or any other issues.

A. The need for further testing and research

1. Alternative fuels for heavy-duty applications

EPA plans to conduct a detailed analysis into the emission benefits of biodiesel fuels. A number of states are considering requirements for biodiesel fuel, and others have programs to promote the use of this fuel. The use of biodiesel is expected to have substantial benefits in reducing carbon dioxide emissions and it may also reduce particulate emissions. For these reasons, it is important that we have a better understanding of the emissions effects of varying concentrations of biodiesel, and a better understanding of the effects of biodiesel on engine durability.

Several states are also considering emission reduction programs that make use of emulsions of diesel fuel and water. Use of these emulsions is expected to reduce NOx and particulate emissions. EPA intends to review the emissions and engine durability data currently available on such emulsions to determine if enough data exists to draw conclusions about these topics.

2. Additional test data

The graphs in Section II.E.1 provide a comparison between the fuels in our database and in-use fuels in terms of distributions of fuel property values. These graphs suggest that our database is a good representation of in-use fuels as well as fuels that tend to be cleaner (i.e. lower emitting) than typical in-use fuels. The sulfur distribution of fuels in our database includes those with sulfur levels in the thousands of ppm, which is indicative of current nonroad diesel sulfur levels. In general, then, it does not appear that there are significant gaps in our fuels database, at least for fuels used in current highway CI engines.

However, our database could benefit from additional data on the newest highway engine technologies, nonroad engines, and light-duty vehicles. For instance, injection rate-shaping is becoming a more prominent form of combustion control, and there is some evidence that it will affect the way in which cetane affects emissions (see Section VII.B.2 below). Our database contains only a single engine meeting the 1998 standards, and this was a pre-production engine. Also, future heavy-duty emission standards may drive the use of particulate traps and NOx adsorbers. Engines with this type of aftertreatment have not yet been tested in a carefully controlled program to determine fuel effects on emissions. There are also some technology types that exist in the current fleet of highway vehicles that are not represented well in our database. These include light-heavy duty engines having a total displacement of less than 9.4 liters and which have relatively slow rated speeds of 2100 rpm or less. Although the results of our Unified approach to model development suggests that engine technology type only has a unique impact on fuel/emission relationships in a limited number of cases, the representativeness of the Unified Model for these engine technologies could be verified by collecting additional data.

There is very limited data on nonroad engines and test cycles, and we were therefore unable to derive an independent model applicable to nonroad engines. As discussed in more detail in Section IV.E, we believe that the default equations for our Unified Model can be applied to nonroad engines. However, it would be useful to collect additional data on nonroad engines to verify that the emission effects exhibited by the equations presented in Section IV.E are in fact representative of nonroad engines under typical nonroad operating conditions. Additional nonroad testing should include not only a wide distribution of diesel fuel properties and engines, but also different test cycles.

Finally, our review of available data indicated that information on toxics impacts of changes in diesel fuel and diesel fuel effects on light-duty vehicles is very limited. These are both areas is which additional test data would be very useful. Until substantial additional test data is collected, we can draw only general conclusions about the way that diesel fuel properties affect toxics emissions from heavy-duty engines and emissions of regulated pollutants from light-duty vehicles.

B. Technical issues in model development

Throughout our analysis, a number of technical issues arose that warrant further investigation. We would welcome comment on these or any other issues.

1. Natural cetane and additized cetane

Our current modeling efforts utilize two distinct cetane terms: natural cetane and delta, or additized, cetane. This was done for a number of reasons, which were discussed in Section II above. There are a number of reasons why one would expect that both natural and additized cetane would impact diesel engine emissions in the same fashion. One, cetane is an indication of ignition delay. If ignition delay affects emissions, then changing ignition delay, whether through modifying the chemical composition of the hydrocarbons in the fuel (natural cetane) or by adding a cetane improver, might be expected to have the same emission impact. Two, several fuel-emission studies have evaluated the effect of changes in both natural and additized cetane on emissions and concluded that they are similar, particularly with respect to NOx and PM emissions.

The Unified Model for PM emissions contains coefficients for both natural and additized cetane and these coefficients are very similar in magnitude. Thus, the general expectation described above is met for PM emissions. However, this is not the case with the NOx emissions model. The Unified NOx emission model only contains a coefficient for delta (additized) cetane. The coefficient for natural cetane was dropped due to the fact that it did not meet the 5% significance level. In fact, it was highly non-significant after the final mixed model regression, with a p-value of 0.88. This dramatic difference in the impact of natural and additized cetane in the Unified NOx model is an issue which we wish to highlight.

a. Review of studies

The first question in addressing this issue is how robust were the conclusions in various studies that natural and additized cetane had the same impact on NOx emissions. We reviewed a number of studies which made this conclusion and our reviews are summarized below.

One study, by Navistar International and Amoco Oil Co., measured the emission impacts of natural cetane and additized cetane, as well as changes in total aromatics and polynuclear aromatics.[24] Four statistical NOx emissions models were developed just for this study's data, two with total aromatics as one of the fuel variables and two with PNAs as one of the fuel variables. The models with total aromatics produced much better correlation, so they will be the focus here.

One of the two models with total aromatics also included delta, or additized cetane, while the other included total cetane (natural plus delta cetane). The cetane term was statistically significant in both cases and the coefficients were essentially identical. However, the model with final cetane showed a 20% lower impact of aromatics on NOx emissions than the model with delta cetane. Neither emission model included specific gravity. We reviewed the fuels tested and found that specific gravity changed substantially between fuels and the change was highly correlated with total aromatics. Natural cetane was also quite correlated with aromatics and specific gravity.

It appears that there are at least two difficulties in using the results of this study to determine that natural and additized cetane have the same impact on NOx emissions. One, natural cetane was never used as a variable in any of the models. Two, natural cetane did not vary independently of other important fuel variables. The fact that total cetane and additized cetane have the same impact in the two models is not surprising, given the high degree of correlation in the study's fuels between aromatics, specific gravity and natural cetane. The difference in the predicted impact of aromatics on NOx emissions with a change in the cetane term is probably due to this correlation. Given that the changes in delta cetane were done in isolation of changes to other fuel parameters, the statistical model found it most efficient to develop the final cetane coefficient almost exclusively from the delta cetane effect. The changes in natural cetane then reduced the changes in NOx emissions assignable to aromatics, so the effect of aromatics decreased.

This study also directly measured the impact of fuels on a number of combustion related parameters, such as ignition delay, premix combustion fraction, and rate of pressure rise. In general, these combustion parameters were highly correlated with cetane, either natural or additized. Thus, at least in terms of engine operation, it does not appear to matter whether fuel cetane comes from the primary fuel hydrocarbons or additives.

A second study by Navistar and Amoco tested a second set of twelve fuels. Natural cetane and aromatics were less correlated in this set. Natural cetane and specific gravity were also not strongly correlated. The best correlations of NOx emissions with fuel properties showed that the effect of both natural and additized cetane were statistically significant. Both aromatics and API gravity were included in this correlation. The effect of natural cetane was roughly 80% that for additized cetane. It seems likely that the confidence intervals for the two cetane coefficients overlap. Thus, the conclusions of this second Navistar-Amoco study appear to more strongly support an equivalent natural-additized cetane effect on NOx emissions.

The CRC VE-1 test program also attempted to estimate the impact of natural and additized cetane on emissions. SwRI, for CRC, developed a number of statistical models for the relationship between fuel properties and NOx emissions. A number of these models included terms for both the logarithm of natural and additized cetane. Both cetane terms were statistically significant and the effect of natural cetane was roughly 50% larger than that for additized cetane.

However, like the first Navistar-Amoco study, natural cetane was highly correlated with specific gravity (Pearson coefficient of -0.80) and specific gravity was not included in the model. Thus, the coefficient for natural cetane likely included a portion of the effect of lower specific gravity and a direct comparison of the two cetane terms cannot be made.

Given the fact that our models show that specific gravity affects NOx and PM emissions substantially, this means that a significant fuel effect was not included in the statistical model and likely affected the calculated emission effects assigned to the other fuel parameters, including the two cetane measures. The changes in specific gravity were most closely associated with total aromatics. The changes in specific gravity were not very associated with changes in natural cetane and totally unrelated to changes in additized cetane. Thus, the absence of specific gravity in this study's emission model is not likely to have affected the calculated emission effects for natural and additized cetane and we found no reason to qualify this conclusion.

A follow-on CRC study, VE-10[m], evaluated the effect of aromatics, natural cetane and additized cetane on two engines, both of which were tested at two NOx emission calibrations. The changes in aromatics, specific gravity, natural cetane and additized cetane were intended to be independent of the others, though there was still significant correlation between aromatics and natural cetane (Pearson coefficient of 0.68). While the potential for comparing the impacts of the two cetane types on NOx emissions exists, the final report for this study did not present NOx emission correlations with natural cetane, additized cetane, and aromatics at the same time. Thus, it is not possible to determine if this study found similar NOx emission impacts for the two types of cetane when the effect of aromatics is separately accounted for.

Some of the most convincing conclusions regarding the relative NOx impact of natural and additized cetane come from the Heavy-Duty Engines Workgoup (HDEWG). In their test program, two sets of two fuels were tested where the pairs of fuels truly differed by only the existence of a cetane improver additive; the aromatics, density, and other fuel properties were nearly identical for each fuel pair. Only two repeat tests were performed on each fuel/engine combination, making the statistical analyses "extremely limited." Even so, the report's authors concluded that natural and additized cetane produce indistinguishable emission effects. We note that the cetane index values were also nearly identical for the pairs of fuels, as were the hydrogen-to-carbon ratios. If NOx is driven by the adiabatic flame temperature as suggested by one stakeholder (see Section VII.B.2), we would expect these two fuels to combust similarly and thus produce the same impact on emissions. The limited dataset produced by the HDEWG does not permit us to prove that natural and additized cetane have different impacts on emissions.

b. Evaluation of Unified Model approach

The second question which could be asked is why our Unified NOx emission model did not find the same NOx emission effects for the two cetane terms. We reviewed the impact of the two cetane terms on NOx emissions in all of the various types of models which we generated. The NOx models for individual technology groups showed a variety of results for the two cetane terms. The mixed NOx models for the two technology groups containing the largest amount of data, F-DD and T, show very similar coefficients for natural and additized cetane. Thus, two large subsets of the database indicate a similar NOx impact for the two types of cetane. However,

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[m] This program was also summarized in SAE papers 941020, 950250, and 950251. The statements made here also apply to the analyses presented in these SAE papers.

these mixed models did not include engine-by-fuel interactive terms, while the Unified Models were developed including these terms..

The Unified Model was not developed without engine-by-fuel interactive terms, however the technology group T model was also developed with these interactive terms. When these terms were included in the mixed NOx model for technology group T, the coefficients for additized cetane and additized cetane squared were statistically significant. However, neither the natural cetane, nor natural cetane squared terms were statistically significant. Of the two, the natural cetane squared term was the more significant (p=0.07), but indicated that increasing cetane increased NOx emissions. Thus, at least for technology group T representing greater than half of the data in the database, the model structure of the mixed model had a significant impact on the predicted effect of natural cetane on NOx emissions.

The NOx model developed using the eigenvector technique found natural and additized cetane effects which were similar to those found by the fixed effect Unified Model. Again, this may not be surprising given that the final modeling step in the eigenvector technique did not include the engine-fuel interactive terms.

While a Unified NOx model was not developed without the engine-by-fuel interactive terms, the fixed effects model which was used to develop a set of candidate fuel-related terms for the mixed model was developed without engine-by-fuel interactive terms. This fixed effects NOx model found that the coefficients for both natural and additized cetane were statistically significant, with the coefficient for additized cetane being about twice as large as that for natural cetane. When the statistically significant terms contained in the fixed effects model were input into a mixed effects model, the additized cetane term was essentially unaffected, while the coefficient for natural cetane dropped in magnitude substantially and ceased to be statistically significant.

It seems clear that the structure of the statistical model used to develop the NOx emission model has a significant impact on the emission effects assigned to natural cetane. The differing projections for the effect of natural cetane may be due to differences in the way the various models separate the effects of natural cetane, specific gravity and aromatics, which are somewhat correlated in the fuels which have been tested to date. We request comment on the issue of relative NOx impacts of natural versus additized cetane, and on the impact that the regression modeling approach may have on these relative effects.

2. Engine sensitivity to cetane

Historically, cetane number has been considered to be one of the most important diesel fuel properties in terms of its impact on engine performance and emissions. Since it is a measure of the combustion properties of the fuel (rather than a strict measure of the fuel's composition or physical properties), there is an expectation that it will interact with engine technology in terms of the impact on emissions. In fact, of all the fuel property effects in our Unified Model which were technology group-specific, cetane arose most frequently.

Our database included data collected on a single engine equipped with exhaust gas recirculation (EGR). This engine was tested as part of the Heavy-Duty Engines Workgroup in an effort to determine how changes in fuel properties would affect emissions from an engine designed to meet the 2004 standards. That study concluded that the EGR-equipped engine actually exhibited a small increase in NOx emissions with increased cetane. We therefore felt it important to create a technology group for EGR-equipped engines (technology group L) so that any effects of cetane on emissions which were significantly different from those for other engine technologies would be captured in our modeling process. In fact, technology group L did have its own adjustment term for additized cetane in our final Unified Model, confirming the findings of the Heavy-Duty Engines Workgroup.

Recently, one stakeholder suggested that the increase in NOx associated with higher cetane levels as observed by the Heavy-Duty Engines Workgroup may not be associated with EGR specifically, but rather with the predominance of diffusion burning that is more characteristic of newer engines. The more frequent use of injection rate-shaping in recent model years to control the combustion process may result in less pre-mix burning, which would raise the adiabatic flame temperature. The result would be that increases in cetane would actually increase NOx emissions. In support of this possible explanation for the unique cetane effects we observed for technology group L, the stakeholder directed us to a combustion simulation model developed by Southwest Research Institute called ALAMO_ENGINE[25]. According to the stakeholder, this model shows no effect of cetane on NOx emissions for engines using rate-shaping.

There is currently insufficient information to determine conclusively whether this explanation is accurate. Aside from additional testing, we could more thoroughly investigate the engines in our database to determine which ones included rate-shaping, and adjust our technology group definitions accordingly. Information about rate-shaping is unlikely to have been presented in the studies from which we derived the data for our database, so this process might require us to contact manufacturers. We request comment on the possibility that rate-shaping, rather than EGR, is the reason that technology group L exhibits a different NOx response to cetane than other technology groups, and on approaches we could take to resolve the issue.

3. Fuel term elimination process in PCR

In applying principle components regression (PCR) to our database, we followed the description given in the DOE report. This analysis is described in Section III.B.1. However, recent communications from the authors suggest that the procedure for eliminating or "pruning" eigenvectors and individual fuel terms which was summarized in the report may not be the actual procedure that the authors actually used. If a change in the pruning procedure were made, it might affect the results of our own PCR analysis.

According to the report's authors, the revised pruning procedure differs from the example in the report in that the eigenvector contributions are summed before squaring, rather than the reverse process shown in the example, thereby retaining the contributions from cross-product terms. Thus while both approaches take the same model sums of squares and apportion part to each fuel term, the apportionment differs between the methods. The revised method uses the squares and cross-product terms of the eigenvector values in determining the individual fuel sums of squares, while the first method uses only the squares of the eigenvector values. We will be investigating the effect that this change would have on our own analysis. In the meantime, we would welcome comments on this issue.

4. Model-year analysis

As discussed in Section II.C, we subdivided our database into technology groups that we believed had the potential for exhibiting different fuel property/emission effects. We chose not to separate the data according to the model year of the engines, because this approach would be less efficient in capturing the different types of engine technologies. In addition, our technology group definitions did correlate roughly with model year, as described in Section II.E.3.

Even so, one stakeholder suggested that categorizing our database by model year might provide a emissions model that is more representative of the in-use fleet. Unfortunately, the selection of engines on our database is not comprehensive enough to permit a model year by model year analysis. There are some model years entirely missing from our database (e.g. 1992, 1997), and other model years consist of only a single engine. Given that so few technology groups had adjustment terms in our Unified Model, we concluded that most engines respond in a similar fashion to changes in diesel fuel properties, and thus we do not consider the absence of data on a few model years to be problematic.

Another reason to avoid a model-year analysis of our database is that there is some ambiguity in how the model years for specific engines are assigned. Many test programs used engines that were designed to meet standards that applied in a particular timeframe (for instance, an engine was designed to meet the standards which apply to 1991 - 1993 model years). An engine described in this way could be assigned to the 1991, 1992, or 1993 model year. Other test engines were actually modified to meet a more stringent set of standards, such that the actual model year of the engine was not really descriptive of the intended model year.

Still, there is some belief that the emission standards to which an engine was certified may provide a unique description of how engines respond to changes in diesel fuel properties. Even though there is a significant distribution of technologies within any given model year, they all have the common attribute of being designed to meet the same emission standards[n]. Thus it may be possible to group engines together according to the emissions standards they were designed to

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[n] Phase-in of emission standards not withstanding.

meet, and to re-apply our Unified approach to this alternatively subdivided database. We request comment on this potential approach and on the expected representativeness of the resulting model.

5. Uncertainty analysis

After the development of any regression-based emissions model, it is prudent to further evaluate the uncertainty associated with the model coefficients. There are a number of ways that such an evaluation can be made. One way would be to determine how well the model can predict fuel effects on emissions for an independent data set. Since we used all available data in the development of our model, this was not possible. An alternative approach could have been to develop the model on the basis of a randomly-chosen subset of the database, and then use the remaining observations to evaluate the model. This approach means that the model will not be based on all available data, and the coefficients could potentially vary depending on the randomly selected observations that are used to construct the model. However, this remains a valid approach to evaluating regression-based emission models, and we request comment on its use for our Unified Model.

Another approach would be to assign error bounds to the regressions equations. In the context of the multivariable mixed model regression that we carried out, determining such error bounds would be very difficult. At best, an estimate of the error bounds could be constructed. However, given that the terms in our final model are there because they are statistically significant, such estimated error bounds are unlikely to indicate that a term should be dropped from the model. Estimated error bounds could, however, provide a degree of confidence that the true effect of changes in fuel properties on emissions lies somewhere within those bounds. In terms of predicted emission effects, then, estimated error bounds will permit one to estimate the likely minimum and maximum emission effects for a given set of fuel properties. We request comment on the need for estimated error bounds and the best way to make use of them in predicting emission effects for the in-use fleet.

Another approach is to carry out a residuals analysis. A residuals analysis provides information on how well the model predicts emission effects for the data on which the model was based. Predicted emissions are compared to observed emissions to ensure that the comparison averages out to 1:1 and that scatter is at a minimum. Since the engine has a much more significant effect on emissions than fuel properties, care must be taken to separate out the engine effects in this process. The most straightforward way to do this is to use the version of the final model that includes intercepts for every engine. SwRI did such an analysis for our final Unified Model and confirmed that the predicted and observed emissions were very similar. See the SwRI report[10] for further details.

Since we intend to use our Unified Model to predict emission effects for the entire fleet rather than for individual engines, we generally ignore the engine intercepts terms. However, doing so may raise the question of how well our Unified Model, sans engine intercepts, predicts the data in our database. Thus it seemed prudent to us to conduct an uncertainty analysis akin to a more traditional residuals analysis, but using percent changes in emissions rather than absolute change in g/bhp-hr. In this analysis, a baseline fuel was chosen from among those tested on each engine in our database, and the percent change in emissions was calculated for the remaining fuels tested on that engine. This approach effectively eliminates the engine effect on emissions, and resembles the manner in which we intend our Unified Model to be used. We then used the same baseline fuel for each engine to calculate the predicted percent change in emissions for each remaining fuel according to our Unified Model sans engine intercepts. The difference between the predicted percent change values from our model and the calculated percent change values from the database was then determined. The results of this analysis are shown in Table VII.B.5-1 (details can be found in the SwRI report[10]).

Table VII.B.5-1
Unified Model predicted versus calculated percent change values

Maximum difference between predicted and calculated percent change values	Cumulative percent of database observations			
	NOx	PM	HC	HC limited†
2	63	23	8	11
4	86	41	16	21
6	95	60	24	29
20	100	98	63	74
30	100	100	82	87
100	100	100	99	100

† The "HC limited" analysis was intended to look more closely at predicted versus observed HC results by limiting the observed values to those that were between -20 and +20 percent change from the baseline fuel

For our NOx model, 86 percent of the observations in the database exhibited a percent change from baseline fuel that differed from the change predicted by our Unified Model by 4 percent or less. Our PM model was less accurate at predicting the effects in the database, but still came within 20 percent of the measured effect 98 percent of the time. Our HC model was a rather poor predictor of the effects in our database.

Note that only the default models from our Unified Model were used in this analysis. Presumably if the individual technology group models had been included, the differences between predicted and calculated percent change values would have been smaller. Also, the fact that the PM model appears to be less accurate than the NOx model, and the HC model less accurate than the PM model, can be partially explained by the relative magnitude of the predicted effects between the three pollutant models for a single fuel. For instance, the default PM model will on average predict percent change effects that are two times larger than those predicted by the default NOx model for the same set of fuel properties. The HC model will on average predict percent change effects that are five times larger than those predicted by the default NOx model. The larger the predicted effects, the wider the error can be while maintaining a statistically significant result. We request comment on this analysis and on the uncertainty associated with predictions made by the Unified Model.

6. Fuel effects on nonroad engines

Although we believe that our Unified Model can provide reasonable predictions of fuel effects for nonroad CI engines, there are several issues that we believe should be addressed. These include differences in the distribution of technology between highway and nonroad engines, and cycle effects. Both of these issues are discussed below. We welcome comments on these or any other issues related to the application of our Unified Model to the nonroad CI fleet.

As discussed in Section IV.E, the Unified Model contained only a few technology group adjustment terms out of the approximately 140 possible. This result lead us to conclude that, with rare exceptions, engine technology does not play a significant role in the relationship between fuel properties and emissions. As a result it seemed appropriate to apply the Unified Model to nonroad engines, since the technology groups we defined in Appendix D could be used to categorize nonroad engines as well as highway engines.

However, we did not take into account the degree to which the distribution of technologies among the nonroad fleet may be different than that for the highway fleet. For instance, the nonroad fleet has a higher proportion of mechanically-controlled engines and indirectly-injected engines than there is in the highway fleet. The range of rated horsepower is also considerably wider for nonroad CI engines. In addition, although there are nonroad engines which exactly mimic highway heavy duty counterparts, some nonroad engines have niche applications that operate under extreme conditions and so have been calibrated to function differently. We have not evaluated the degree to which these types of differences in engine technology between nonroad and highway engines could affect correlations between diesel fuel properties and emissions. In large part this is due to the fact that the available data on fuel effects for nonroad engines is extremely limited. In the coming months we will be attempting to validate the use of the Unified Model for nonroad using recently collected data on nonroad engines. In the interim, because nonroad engine technology tends to follow highway engine technology, though lagging by a few model years, and our Unified Model did not appear to have a strong technology component, we have proposed that the Unified Model for NOx and HC be used to represent nonroad as well as highway engines.

A potentially more significant difference between highway and nonroad engines is the way in which they are operated, and thus the duty cycles that are most representative. In our current effort for highway vehicles, we have based our models on emission data collected with test cycles that are intended to represent highway operation. In general these included both transient and steady-state cycles, though the PM model was based only on testing with the transient highway

FTP (as explained in Section II.D.3). As described above, there was simply insufficient data on nonroad engines using nonroad engine cycles. However, we suggest that highway cycles can serve as a basis for comparison and extrapolation to nonroad applications for relative effects of fuel property changes on emissions. We believe this is appropriate because the Unified Model is based on both transient and steady-state test data, and the variety of cycles being evaluated for nonroad include both transient and steady-state. To appropriately characterize PM impacts it may be necessary to build up a database which incorporates additional transient nonroad cycle data once a sufficiently robust data set becomes available.

EPA has a steady-state certification test for nonroad engines. Given the paucity of nonroad data, we do not believe that this fact is sufficient to conclude that the Unified Model, which includes transient test data, is not representative of nonroad. However, we could later revise our Unified Model for application to nonroad if sufficient additional data is collected. We welcome comment on whether the potential cycle differences between highway and nonroad would affect the applicability of the Unified Model to nonroad.

7. Monoaromatic versus polyaromatic effects

As discussed more fully in Section III.C.1, we chose to use total aromatics in our modeling effort instead of monoaromatics and polyaromatics. If we had included monoaromatic and polyaromatic terms in our stepwise regression, we would have lost over 50% of the data in our database. This is a significant amount of data to lose, and the model could potentially have exhibited different fuel property/emissions correlations as a result. Thus we determined that it was more reasonable to include only a total aromatic term for our draft model than to lose 50% of the available data. However, there may be statistical methods, such as correlation partialling, that would permit the development of a regression model that bases the effects of mono and polyaromatics on a subset of the database, while the remaining fuel properties are based on the entire database. We have not investigated this type of approach. We request comment on whether and how to include the separate effects of monoaromatics and polyaromatics in our modeling.

Appendices

Appendix A - Data Sources

<u>Data sources which meet all basic criteria and which were included in the database</u>

1. Mitchell, K., "Effects of Fuel Properties and Source on Emissions from Five Different Heavy Duty Diesel Engines," SAE 2000-01-2890

2. Cheng, A. S., R. W. Dibble, “Emissions Performance of Oxygenate-in-Diesel Blends and Fischer-Tropsch Diesel in a Compression Ignition Engine,” SAE 1999-01-3606.

3. Schwab, Scott D., G. H. Guinther, T. J. Henly, K. T. Miller, “The Effects of 2-Ethylhexyl Nitrate and Di-Tertiary-Butyl Peroxide on the Exhaust Emissions from a Heavy-Duty Diesel Engine,” SAE 1999-01-1478.

4. Clark, Nigel N., C. M. Atkinson, G. J. Thompson, R. D. Nine, “Transient Emissions Comparisons of Alternative Compression Ignition Fuels,” SAE1999-01-1117.

5. Starr, Michael E., “Influence on Transient Emissions at Various Injection Timings, Using Cetane Improvers, Bio-Diesel, and Low Aromatic Fuels,” SAE 972904.

6. Schabert, Paul W., Ian S. Myburgh, Jacobus J. Botha, Piet N. Roets, Carl L. Viljeon, Luis P. Dancuart, Michael E. Starr, “Diesel Exhaust Emissions Using Sasol Slurry Phase Distillate Process Fuels,” SAE 972898.

7. Lange, W.W., J.A. Cooke, P. Gadd, H.J. Zurner, H. Schlogl, and K. Richter., “Influence of fuel Properties on Exhaust Emissions from Advanced heavy-Duty Engines considering the Effect of Natural and Additive Enhanced Cetane Number,” SAE 972894.

8. Stradling, Richard, Paul Gadd, Meinrad Signer, Claudio Operti, “The Influence of fuel Properties and Injection Timing on the Exhaust Emissions and fuel Consumption of an Iveco Heavy-Duty Diesel Engine,” SAE 971635.

9. Tamanouchi, Mitsuo, Jiroki Morihisa, Shigehisa yamada, Jihei Lida, Takanobu Sasaki, and Harufusa Sue, “Effects of Fuel Properties on Exhaust Emissions for Diesel Engines With and Without Oxidation Catalyst and High Pressure Injection,” SAE 970758.

10. Daniels, Teresa L., Robert L. McCormick, Michael S. Graboski, Philip N. Carlson, Venkatesh Rao, and Gary W. Rich, “The Effect of diesel Sulfur Content and Oxidation Catalysts on Transient Emissions at High Altitude from a 1995 Detroit diesel Series 50 Urban Bus Engine,” SAE 961974.

11. Geiman, Richard A., Patrick B. Cullen, Peter R. Chant, Philip N. Carlson and Venkatesh Rao, “Emission Effects of Shell LOW NOX Fuel on a 1990 Model Year Heavy Heavy-Duty Diesel Engine,” SAE 961973.

12. Signer, M., P. Heinze, R. Mercogliano, H.J. Stein, "European Programme on Emissions, Fuels and Engine Technologies (EPEFE) - Heavy-Duty Diesel Study," SAE 961074

13. Mitchell, K., D.E. Steere, J.A. Taylor, B. Manicom, J.E. fisher, E.J. Sienicki, C. Chiu, P. Williams, “Impact of Diesel Fuel Aromatics on Particulate, PAH and Nitro-PAH Emissions,” SAE 942053.

14. Nandi, Manish K., David C. Jacobs, Frank J. Liotta, Jr., H.S. Kesling, Jr., “The Performance of a Peroxide-Based Cetane Improvement Additive in Different Diesel Fuels,” SAE 942019.

15. Rosenthal, M. Lori, Tracy Bendinsky, “The Effects of Fuel Properties and Chemistry on the Emissions and Heat Release of Low-Emission Heavy Duty Diesel Engines,” SAE 932800.

16. Liotta, Jr., Frank J., “A Peroxide Based Cetane improvement Additive with Favorable Fuel Blending Properties,” SAE 932767.

17. Liotta, Jr., Frank J., Daniel M. Montaivo, “The Effect of Oxygenated Fuels on Emissions from a Modern Heavy-Duty Diesel Engine,” SAE 932734.

18. Gonzalez D., Manuel A., Guillermo B. Rodriguez, Roberto Galiasso, Edilberto Rodriguez, “A Low Emission Diesel Fuel: Hydrocracking Production, C haracterization and Engine Evaluations,” SAE 932731.

19. Lange, W.W., A. Schafer, A. Le’Jeune, D. Naber, A.A. Reglitzky, M. Gairing, “The influence of Fuel Properties on Exhaust Emissions from Advanced Mercedes Benz Diesel Engines,” SAE 932685.

20. McCarthy, Christopher I., Warren J. Slodowske, Edward J. Sienicki, Richard E. Jass, “Diesel Fuel Property Effects on Exhaust Emissions from a Heavy Duty Diesel Engine that Meets 1994 Emissions Requirements, SAE 922267.

21. Asaumi, Y., M. Shintani, Y. Watanabe, "Effects of Fuel Properties on Diesel Engine Exhaust Emission Characteristics," SAE 922214 (raw data provided by author)

22. Lange, W.W., “The Effect of Fuel Properties on Particulates Emissions in Heavy-Duty Truck Engines Under Transient operating Conditions,” SAE 912425.

23. Ullman, Terry L., David M. Human, “Fuel and Maladjustment Effects on Emissions from a Diesel Bus Engine,” SAE 910735.

24. Cunningham, Lawrence J., Timothy J. Henly, Alexander M. Kulinowski, “The Effects of Diesel Ignition Improvers in Low-Sulfur Fuels on Heavy-Duty Diesel Emissions,” SAE 902173.

25. Sienocki, E., R.E. Jass, W.J. Slowdowske, C.I. McCarthy, A.L. Krodel, "Diesel Fuel Aromatic and Cetane Number Effects on Combustion and Emissions from a Prototype 1991 Diesel Engine," SAE 902712

26. Knuth, Hans Walter, Hellmut Garthe, “Future Diesel Fuel Compositions - Their Influence on Particulates.” SAE 881173.

27. Barry, E.G., L.J. McCabe, D.H. Gerke, J.M. Perez, “Heavy-Duty Diesel Engine/Fuels Combustion Performance and Emissions - A Cooperative Research Program,” SAE 852078.

28. Hare, C.T., R.L. Bradow, "Characterization of heavy-Duty Diesel Gaseous Particulate Emissions, and Effects of Fuel Composition," SAE 790490

29. Ullman, Terry L.,”Investigation of the Effects of Fuel Composition and Injection and Combustion System Type on Heavy-Duty Diesel Exhaust Emissions,” CRC Contract CAPE 32-80. Project VE-1.

30. Ullman, Terry L., R. L. Mason, D. A. Montalvo, “Study Of Fuel Cetane Number And Aromatic Content Effects on Regulated Emissions From A Heavy-Duty Diesel Engine,” CRC Contract NO. VE-1. Project VE-1.

31. Spreen, Kent B., T. L. Ullman, R. L. Mason, “Effects of Fuel Oxygenates, Cetane Number, and Aromatic Content on Emissions From 1994 and 1998 Prototype Heavy-Duty Diesel Engines,” CRC Contract No. VE-10. Project VE-10.

32. Matheaus, Andrew C., T. W. Ryan III, R. Mason, G. Neely, R. Sobotowski, “Gaseous Emissions From A Caterpillar 3176 (With EGR) Using A Matrix of Diesel Fuels (Phase 2),” Final Report under EPA Contract Number 68-C-98-169, September 1999.

33. Fritz, S.G., "Diesel Fuel Effects on Locomotive Exhaust Emissions," Southwest Research Institute Final Report, prepared for California Air Resources Board in October, 2000.

34. Kleinschek, G., K. Richter, A. Roj, M. Signer, H.J. Stein, "Influence of Diesel Fuel Quality on Heavy-Duty Diesel Engine Emissions," ACEA Heavy-Duty Diesel Truck Manufacturers, March 20, 1997, VE/ACEA/30.

35. Treux, Timothy J., J.M. Norbeck, M.R. Smith, "Evaluation of Factors That Affect Diesel Exhaust Toxicity," report sponsored by the California Air Resources Board, July 24, 1998

Data sources which met all criteria, but the data was not readily available

1. Vertin, K. D., J. M. Ohi, D. W. Naegeli, K. H. Childress, G. P. Hagen, C. I. McCarthy, A. S. Cheng, R. W. Dibble, “Methylal and Methylal-Diesel Blended Fuels for Use in Compression-Ignition Engines,” SAE 1999-01-1508.

2. Uchida, M., Y. Akasaka, "A Comparison of Emissions from Clean Diesel Fuels," SAE 1999-01-1121

3. Tamanouchi, M., H. Morihisa, H. Araki, S. Yamada, "Effects of Fuel Properties and Oxidation Catalyst on Exhaust Emissions for Heavy-Duty Diesel Engines and Diesel Passenger Cars," SAE 980530

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    Reason: Only two modes tested.

Appendix B - Database Structure

Table B1 - File Definitions

File Name	Definition
EQUIP_AD	This table represents the procurement of both Equipment and Engine for the engine tests.
ETEST_AD	Any observation, measurement, or modification to a mobile source. This entity stores the results of an engine test performed on an engine dynamometer.
FBAT_AD	A particular batch of fuel that can be used to power mobile sources during emission tests. Instances of this entity represent a physical batch of fuel that has measured properties.

Table B2 - Individual field definitions

File Name	Field	Definition
EQUIP_AD	eng_ms_id	Mobile source identifier. For engines, their serial number, probably in conjunction with their manufacturer code.
	study_id	Identification number assigned to the analysis/paper/report of interest.
	veh_ms_id	Mobile source identifier. For equipment this would be the serial number which best identifies the equipment as a whole. .
	vehclass	vehicle class. Will have a translation table. Values defined by translation table for this field.
	vehcompany	Vehicle manufacturer. Is designed to align with the MFR_ fields in CFEIS. Has extended translation table in which COMPANY_N will contain the same numeric code as CFEIS for this manufacturer. Values defined by Company translation table for this field.
	engcompany	Engine manufacturer. Is designed to align with the MFR_ fields in CFEIS. Has extended translation table in which COMPANY_N will contain the same numeric code as CFEIS for this manufacturer. Values defined by Company translation table for this field.
	highway	Yes if mobile source is intended for highway use. No for non-road mobile sources.
	model_name	model name
	model_yr	If a prototype, enter representative model year.

File Name	Field	Definition
	make	Vehicle make e.g. Buick, as distinct from vehicle manufacturer, GM. Legal values defined by MAKE translation table. Values defined by translation table for this field.
	disp_liter	Nominal engine displacement, expressed in liters.
	fi_type	type of fuel injection PFI (port fuel injection) TBI (throttle body injection) INDIR (Indirect injection) DIRECT (direct fuel injection e.g. as for most diesel engines.) Values defined by translation table for this field.
	aspirated	indicates how engine is aspirated. CHARGED if turbocharged or supercharged. NATURAL if not. Values defined by translation table for this field.
	cylinder	Number of cylinders or rotors.
	cat_type	What type catalyst, if any, is present on the mobile source. Values are: 3WAY Three-way catalyst OX3W Oxidation plus three-way catalyst OXID Oxidation Catalyst NONE No catalyst NULL Unknown Values defined by translation table for this field.
	egr_type	Type of exhaust gas recirculation (EGR). Values defined by translation table. Values defined by translation table for this field.
	engseries	Engine series or product line name.
	cooling	Type of after_cooling. (Legal values defined by translation table.) Values defined by translation table for this field.
	fi_meth	Method of fuel injection. (Legal values defined by translation table.)
	fi_press	Fuel injection pressure, expressed in kPa.
	parttrap	Is particulate trap used? "YES", "NO", or "NUL".
	eng_cycle	Engine cycle, 2 =. 2-stroke, 4 = 4-stroke. 0 = Unknown. Values defined by translation table for this field.
	ratedpower	Rated horsepower of engine.
	ratedspeed	Rated rpm of engine
	idle_rpm	Idle rpm as declared by the oem.

File Name	Field	Definition
	proc_odom	Approximate odometer reading in miles at time of vehicle recruitment.
	hour_meter	Hours of operation (usually available only for off-road mobile sources). Null value is 0.
	gvwr	Gross vehicle weight rating in pounds. The value specified by the manufacturer as the loaded weight of a single vehicle.
	pk_torque	Peak torque of the engine expressed in ft-lb.
	pk_t_speed	Peak torque speed expressed in rpm.
	cyl_valves	The number of valves per cylinder.
	stroke	Piston stroke expressed in inches. (not ready to be stored in msod database at this time)
	bore	The diameter of the cylinder expressed in inches.
	inj_ctrl	Code of the Injection control type. Values defined by translation table for this field.
	inj_pcat	Code of the injection equipment/pressure category. Values defined by translation table for this field.

File Name	Field	Definition
ETEST_AD	test_id	Identification number assigned to the engine test.
	study_id	Identification number assigned to the analysis/paper/report of interest.
	fbatch_id	Fuel batch identification.
	eng_ms_id	Mobile source identifier. For engines, their serial number, probably in conjunction with their manufacturer code.
	test_proc	Identifies the specific test procedure used. Values defined by translation table for this field.
	ms_type	General kind of mobile source: 1 = Vehicle 2 = Engine.
	No_modes	Number of test modes involved in this result. Data for individual chassis test modes is stored in the DYNOMODE table; data for individual engine dynamometer test modes is stored in the EMODE table.
	p_ch4	Methane emissions. Expressed in grams per bhp-hr.
	p_thc	Total HC emissions. Expressed in grams per bhp-hr.
	p_co	CO emissions. Expressed in grams per bhp-hr.
	p_nox	NOx emissions. Expressed in grams per bhp-hr.
	p_pm	Total particulate emissions. Expressed in grams per bhp-hr.
	total_work	Total work performed in test. Expressed in bhp-hrs.
	bsfc_meas	Measured brake-specific fuel consumption. Expressed in pounds per bhp-hr.

File Name	Field	Definition
FBAT_AD	fbatch_id	Fuel batch identification.
	study_id	Identification number assigned to the analysis/paper/report of interest.
	cetane_num	Cetane number of complete fuel.
	cetane_idx	Cetane index of complete fuel.
	cetane_imp	Amount of cetane improver added, expressed as percentage by volume
	cetane_typ	Type of cetane improver used, e.g. "N" for nitrate type or "P" for peroxide type. Exact set of legal values defined and described by translation table for this field.
	sulfur	Sulfur content, expressed in parts per million.
	nitrogen	Nitrogen content, expressed in parts per million.
	tarom	Total aromatics content of fuel, expressed as a percentage by volume. This is a measured value, as opposed as being calculated as the sum of the monoaromatics and polyaromatics fields.
	marom	Monoaromatics content of fuel, expressed as a percentage by weight. This is a measured value, as opposed as being calculated as the difference of the total aromatics and polyaromatics fields.
	parom	Polyaromatics content of fuel, expressed as a percentage by weight. This is a measured value, as opposed as being calculated as the difference of the total aromatics and monoaromatics fields.
	IBP	Initial boiling point expressed in degrees F.
	T10	10% distillation boiling point, expressed in degrees Fahrenheit.
	T50	50% distillation boiling point, expressed in degrees Fahrenheit.
	T90	90% distillation boiling point, expressed in degrees Fahrenheit.
	T95	95% distillation boiling point, expressed in degrees Fahrenheit.
	EP	End point of distillation curve, expressed in degrees Fahrenheit.
	spec_grav	Specific gravity.
	viscosity	Viscosity, expressed in centistokes @40 degrees F.
	hcratio	Molecular ratio of hydrogen to carbon.
	oxygen	Amount of oxygen in the fuel, expressed as a percentage by weight.

File Name	Field	Definition
	oxy_type	Type of oxygenate. "NONE" if no oxygenate was added to the base fuel. Values defined by translation table for this field.
	heat	Net heating value of the fuel, expressed in btu/pound.
	ash	Ash content of fuel, expressed as a percentage.
	cetane_dif	This is the difference in cetane number between the described fuel (with additive) and a baseline fuel without additive.

Appendix C - Aromatics Conversion Equations

As data was copied from the studies we considered relevant into our database, we made conversions as necessary to ensure that the database represented a consistent set of units. For aromatics, the test method can be just as important as the units, since different aromatics test methods can produce measurements which are biased relative to other aromatics test methods. Thus it was necessary for aromatics values to be entered not only in a consistent set of units, but also representing consistent test methods.

We determined that all total aromatics entries should represent a fluorescent indicator adsorption (FIA) test method such as ASTM D 1319, producing units of volume percent. For mono-aromatics and polyaromatics, we determined that all entries should represent a supercritical fluid chromatography (SFC) test method such as ASTM D 5186, with units of weight percent. These units and test methods were chosen to represent the most common approaches that refiners use to measure aromatics.

As stated in Section II.B.2, we made use of a conversion equation for total aromatics that can be found in the California Code of Regulations, Title 13, Section 2282(c)(1) to convert wt% by SFC to vol% by FIA for total aromatics. However, there were a number of other cases in which a conversion needed to be made but no equation was readily available. For these cases, conversion equations were developed especially for this project.

Throughout the studies that were used to develop our database, there were only two test methods that needed to be converted into units of vol% by FIA for total aromatics or wt% by SFC for mono and polyaromatics. These two test methods were mass spectrometry and high pressure liquid chromatography (HPLC). Available studies were reviewed for cases in which fuels were tested on two different test methods. This data was collected and used to develop correlations between test methods. A summary of the data sources used to develop the correlations is shown in Table C1.

Table C1 - Data sources for aromatics conversion equations

Aromatics component	Conversion from	Conversion to	Data sources	Observations
Total	wt% by mass spec	vol% by FIA	SAE 942053 SAE 2000-01-2980 VE-10 VE-1 Phase 1 VE-1 Phase 2	32
Total	wt% by HPLC	vol% by FIA	SAE 2000-01-2980 SAE 972968 VE-1 Phase 1	21
Mono	wt% by mass spec	wt% by SFC	VE-10 SAE 942053 HDEWG SAE 2000-01-2980	26
Mono	wt% by HPLC	wt% by SFC	SAE 2000-01-2980 SAE 972968	11
Poly	wt% by mass spec	wt% by SFC	VE-10 SAE 942053 HDEWG SAE 2000-01-2980	26
Poly	wt% by HPLC	wt% by SFC	SAE 2000-01-2980 SAE 972968	11

Regression analysis was applied to the data described in Table C1 using linear terms for the aromatics measurements. Specific gravity was included if doing so improved significantly the fit and the data was available. The resulting correlations are shown in Tables C2, C3, and C4, along with the associated R^2 values. These correlations were used to convert the data from the studies we used into the units and test method bases we chose for our database.

Table C2 - Correlations for total aromatics

[vol% by FIA] = 0.777 X [wt% by mass spec] + 132.2 X [sp. gravity] - 105.0	$R^2 = 0.93$
[vol% by FIA] = 0.760 X [wt% by HPLC] + 178.0 X [sp. gravity] - 144.4	$R^2 = 0.96$

Table C3 - Correlations for mono aromatics

[wt% by SFC] = 0.882 X [wt% by mass spec] + 2.37	$R^2 = 0.91$
[wt% by SFC] = 0.885 X [wt% by HPLC] + 0.88	$R^2 = 0.99$

Table C4 - Correlations for poly aromatics

[wt% by SFC] = 1.22 X [wt% by mass spec] + 0.33	$R^2 = 0.95$
[wt% by SFC] = 1.27 X [wt% by HPLC] + 0.69	$R^2 = 0.97$

Appendix D - Technology Groups

Tech Group	Governed speed (rpm)	Injector type	Aspiration	Horsepower	Displacement (L)	Oxy catalyst?	Injection control	Injection type	Cycle	EGR?
A	any	any	Turbo	any	any	No	Mechanical	Direct	Any	Yes
B	any	any	Turbo	any	any	No	Mechanical	Direct	2-stroke	No
C	>3000	unit	Turbo	any	<=9.4	No	Mechanical	Direct	4-stroke	No
D	>3000	inline or rotary	Turbo	any	<=9.4	No	Mechanical	Direct	4-stroke	No
E	<=3000	unit	Turbo	any	<=9.4	No	Mechanical	Direct	4-stroke	No
F	<=3000	inline or rotary	Turbo	any	<=9.4	No	Mechanical	Direct	4-stroke	No
G	2101 - 2500	unit	Turbo	any	>9.4	No	Mechanical	Direct	4-stroke	No
H	2101 - 2500	inline or rotary	Turbo	any	>9.4	No	Mechanical	Direct	4-stroke	No
I	<=2100	unit	Turbo	<500 hp	>9.4	No	Mechanical	Direct	4-stroke	No
J	<=2100	unit	Turbo	>500 hp	>9.4	No	Mechanical	Direct	4-stroke	No
K	<=2100	inline or rotary	Turbo	any	>9.4	No	Mechanical	Direct	4-stroke	No
L	any	any	Turbo	any	any	No	Electronic	Direct	Any	Yes
M	any	any	Turbo	any	any	No	Electronic	Direct	2-stroke	No
N	>3000	unit	Turbo	any	<=9.4	No	Electronic	Direct	4-stroke	No
O	>3000	inline or rotary	Turbo	any	<=9.4	No	Electronic	Direct	4-stroke	No
P	<=3000	unit	Turbo	any	<=9.4	No	Electronic	Direct	4-stroke	No
Q	<=3000	inline or rotary	Turbo	any	<=9.4	No	Electronic	Direct	4-stroke	No
R	2101 - 2500	unit	Turbo	any	>9.4	No	Electronic	Direct	4-stroke	No
S	2101 - 2500	inline or rotary	Turbo	any	>9.4	No	Electronic	Direct	4-stroke	No
T	<=2100	unit	Turbo	<500 hp	>9.4	No	Electronic	Direct	4-stroke	No
U	<=2100	unit	Turbo	>500 hp	>9.4	No	Electronic	Direct	4-stroke	No
V	<=2100	inline or rotary	Turbo	any	>9.4	No	Electronic	Direct	4-stroke	No
W	any	any	any	any	any	No	Electronic	Indirect	4-stroke	No
X	any	any	any	any	any	No	Mechanical	Indirect	4-stroke	No
Y	any	any	Turbo	any	any	Yes	Mechanical	Direct	Any	Yes
Z	any	any	Turbo	any	any	Yes	Mechanical	Direct	2-stroke	No
AA	>3000	unit	Turbo	any	<=9.4	Yes	Mechanical	Direct	4-stroke	No
BB	>3000	inline or rotary	Turbo	any	<=9.4	Yes	Mechanical	Direct	4-stroke	No

CC	<=3000	unit	Turbo	any	<=9.4	Yes	Mechanical	Direct	4-stroke	No
DD	<=3000	inline or rotary	Turbo	any	<=9.4	Yes	Mechanical	Direct	4-stroke	No
EE	2101 - 2500	unit	Turbo	any	>9.4	Yes	Mechanical	Direct	4-stroke	No
FF	2101 - 2500	inline or rotary	Turbo	any	>9.4	Yes	Mechanical	Direct	4-stroke	No
GG	<=2100	unit	Turbo	<500 hp	>9.4	Yes	Mechanical	Direct	4-stroke	No
HH	<=2100	unit	Turbo	>500 hp	>9.4	Yes	Mechanical	Direct	4-stroke	No
II	<=2100	inline or rotary	Turbo	any	>9.4	Yes	Mechanical	Direct	4-stroke	No
JJ	any	any	Turbo	any	any	Yes	Electronic	Direct	Any	Yes
KK	any	any	Turbo	any	any	Yes	Electronic	Direct	2-stroke	No
LL	>3000	unit	Turbo	any	<=9.4	Yes	Electronic	Direct	4-stroke	No
MM	>3000	inline or rotary	Turbo	any	<=9.4	Yes	Electronic	Direct	4-stroke	No
NN	<=3000	unit	Turbo	any	<=9.4	Yes	Electronic	Direct	4-stroke	No
OO	<=3000	inline or rotary	Turbo	any	<=9.4	Yes	Electronic	Direct	4-stroke	No
PP	2101 - 2500	unit	Turbo	any	>9.4	Yes	Electronic	Direct	4-stroke	No
QQ	2101 - 2500	inline or rotary	Turbo	any	>9.4	Yes	Electronic	Direct	4-stroke	No
RR	<=2100	unit	Turbo	<500 hp	>9.4	Yes	Electronic	Direct	4-stroke	No
SS	<=2100	unit	Turbo	>500 hp	>9.4	Yes	Electronic	Direct	4-stroke	No
TT	<=2100	inline or rotary	Turbo	any	>9.4	Yes	Electronic	Direct	4-stroke	No
UU	any	any	any	any	any	Yes	Electronic	Indirect	4-stroke	No
VV	any	any	any	any	any	Yes	Mechanical	Indirect	4-stroke	No
WW	>3000	unit	Natural	any	any	No	Mechanical	Direct	4-stroke	No
XX	>3000	inline or rotary	Natural	any	any	No	Mechanical	Direct	4-stroke	No
YY	<=3000	unit	Natural	any	any	No	Mechanical	Direct	4-stroke	No
ZZ	<=3000	inline or rotary	Natural	any	any	No	Mechanical	Direct	4-stroke	No
AAA	2101 - 2500	unit	Natural	any	any	No	Mechanical	Direct	4-stroke	No
BBB	2101 - 2500	inline or rotary	Natural	any	any	No	Mechanical	Direct	4-stroke	No
CCC	<=2100	unit	Natural	any	any	No	Mechanical	Direct	4-stroke	No
DDD	<=2100	inline or rotary	Natural	any	any	No	Mechanical	Direct	4-stroke	No

References

1. See Clean Air Act § 211(i); 40 CFR § 80.29.

2. See 13 Calif. Code of Regulations, Sections 2281- 2282.

3. See 30 Texas Admin. Code, Chapter 114, Sections 114.6, 114.312-317, 114.319, adopted by the Texas Natural Resource Conservation Commission (TNRCC), April 19, 2000.

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