



# **The Effect of Cetane Number Increases Due to Additives on NOx Emissions from Heavy-Duty Highway Engines**

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

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may form the basis for a final EPA decision, position, or regulatory action.*

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## **I. Introduction**

### **A. Background**

The control of diesel fuel properties as a means for reducing emissions of regulated pollutants continues to be of interest to State air quality managers. Previous test programs have shown various levels of benefits for changes to such fuel properties as cetane number, aromatics, density, sulfur, and distillation properties. For areas that are out of attainment for ozone or particulate matter, State air quality managers may consider changes to diesel fuel as one element of their overall strategy for meeting the National Ambient Air Quality Standards.

One example of a State that has implemented a diesel fuel approach as part of its overall strategy to reach attainment is Texas. When its Low Emission Diesel (LED) program was first proposed for Houston and Dallas in the fall of 2000, EPA voiced concern about the NO<sub>x</sub> emission reduction benefits claimed by Texas. Because of this concern, we initiated an effort to evaluate the emission benefits of varying diesel fuel parameters. In July of 2001, we issued a Staff Discussion Document<sup>1</sup> with the preliminary results of this analysis.

Our process in conducting this evaluation involved reviewing existing engine emissions data rather than conducting new emissions tests. Where data was available, we used a regression model approach to analyze results and to develop a quantitative set of relationships between fuel parameters and emissions changes (in the remainder of this technical report, this work will be referred to as the Staff Discussion Document model). As part of our process, we met with numerous stakeholders to review our preliminary conclusions, beginning in May of 2001, and in response to requests from stakeholders, held a public workshop on August 28, 2001 to hear comments on our Staff Discussion Document and our analysis.

After reviewing the comments made at the workshop, we estimated the NO<sub>x</sub> emission factors for the Texas diesel fuel program based on this analysis. Our conclusions were summarized in a memorandum to EPA's Region VI<sup>2</sup>. In this memorandum, we limited the use of the draft NO<sub>x</sub> model presented in the Staff Discussion Document to the evaluation of the benefits of the Texas diesel fuel program. As a result, there currently exists no widely-applicable, EPA-approved model for estimating the emission impacts of more general changes in diesel fuel properties. At this time, EPA has no plans to pursue such a model.

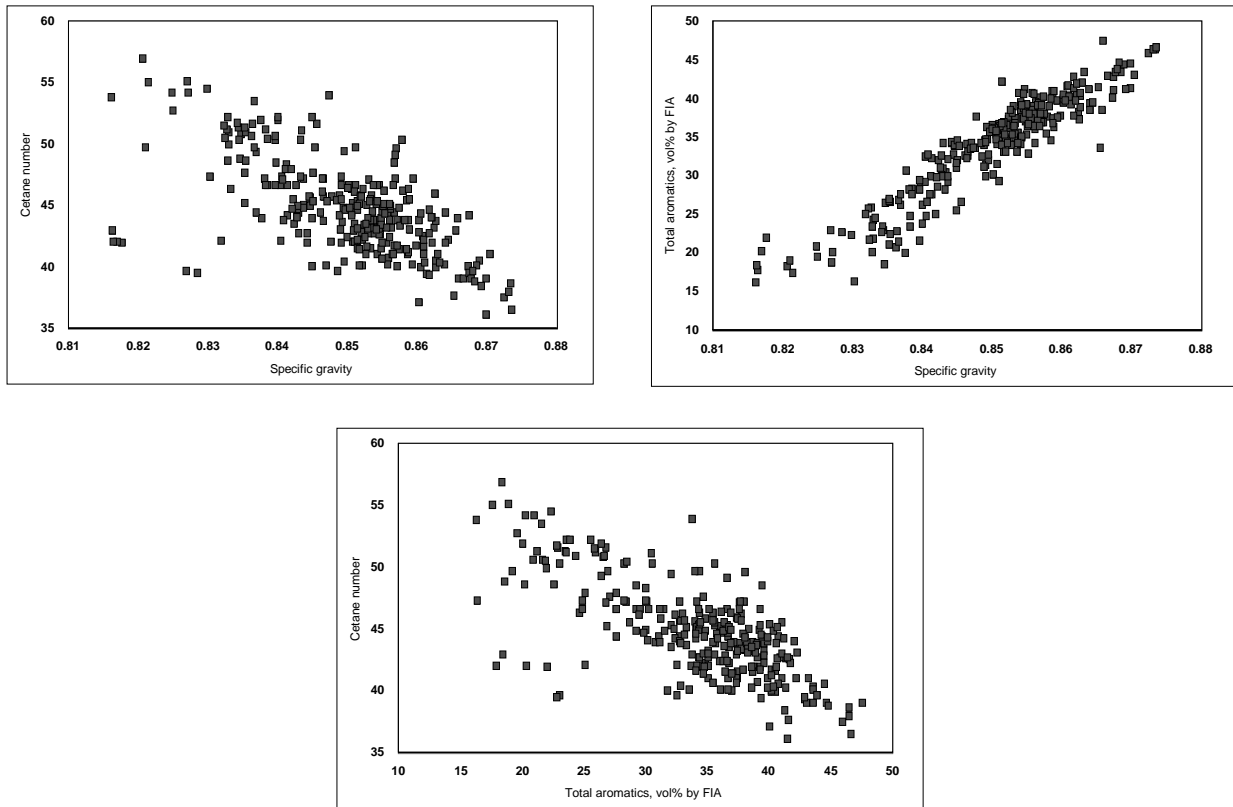
### **B. Cetane number as an emission control strategy**

Of the various diesel fuel properties that could be controlled in order to produce emission benefits, cetane number holds the greatest interest, particularly with regard to NO<sub>x</sub>. Even in the absence of a more comprehensive model correlating all diesel fuel properties with emissions, some States are still considering implementing cetane control programs. In such cases, the emission benefits might be based on results from various individual test programs that attempted

to control cetane number. Since any NO<sub>x</sub> benefits claimed in a SIP as a result of cetane control must eventually be approved by EPA, we have determined that it is now appropriate to investigate the NO<sub>x</sub> benefits of cetane control in a comprehensive fashion.

The cetane number of diesel fuel can be increased in two different ways: naturally, and via the use of additives. The "natural" approach involves the modification of various physical properties of diesel fuel and/or modifying the concentration of various diesel fuel components. The result is that multiple properties/components may change at the same time. This "colinearity" is best illustrated for cetane, aromatics, and specific gravity, as shown in Figure I.B-1<sup>3</sup>.

Figure I.B-1  
Colinearities for natural cetane number



This colinearity can also be seen in variance inflation factors. Variance inflation factors are based on the  $r^2$  value (coefficient of determination) resulting from a least-squares regression in which one fuel property is made a function of all other fuel properties. A value close to 1 indicates that no correlation exists. A value higher than 5 would indicate a moderately strong correlation, while values approaching 10 indicate very strong correlations. A listing of variance inflation factors is shown in Table I.B-1 for in-use survey data.

Table I.B-1  
Variance inflation factors for in-use survey data

Natural cetane	7.1
Additized cetane <sup>α</sup>	1.1
Sulfur	1.3
Aromatics	10.0
T10	4.8
T50	11.1
T90	4.2
Specific gravity	16.7

<sup>α</sup> "Additized cetane" is the increase in total cetane number brought about through the addition of cetane improver additives.

From this table it is clear that natural cetane is highly correlated with other fuel properties. In addition, the high variance inflation factors for aromatics and specific gravity indicate that these three properties are highly correlated with one another (the distillation properties are primarily correlated with each other). However, since fuels in test programs are sometimes the product of more carefully designed blending that might decorrelate fuel properties from each another, the values in Table I.B-1, based on a survey of in-use fuels, may be misleading. We therefore repeated the calculation of variance inflation factors for the Staff Discussion Document model database. The result was that the variance inflation factors were indeed lower than the values in Table I.B-1, but not significantly.

Finally, a correlation matrix is another way to investigate colinearities between fuel properties. Using our emissions database, we generated a correlation matrix by standardizing all of the fuel property measurements (by subtracting the mean from every observation and dividing by the standard deviation), multiplying the fuels matrix by its transpose, and normalizing the results. The results for the primary fuel properties of interest are shown in Table I.B-2. The matrix is necessarily identical on either side of the diagonal.

Table I.B-2  
Correlation matrix for diesel emissions database

	Natural Cetane	Additized cetane	Sulfur	Aro-matics	T10	T50	T90	Specific gravity
Natural Cetane	1							
Additized cetane	-0.35	1						
Sulfur	-0.04	-0.17	1					
Aromatics	<b>-0.57</b>	0.20	0.30	1				
T10	0.16	-0.08	0.01	0.13	1			
T50	0.26	-0.07	0.11	0.30	<b>0.69</b>	1		
T90	0.32	-0.10	0.10	0.23	0.30	<b>0.70</b>	1	
Specific gravity	<b>-0.61</b>	0.25	0.21	<b>0.75</b>	0.30	0.41	0.23	1

As the values in the correlation matrix approach 1 (or -1), the correlation between the two fuel properties in question approaches a perfect linear correlation. Thus the Table I.B-2 values can be viewed as correlation coefficients for one fuel property as a function of another fuel property. The highest values are for T50 as a function of the adjacent distillation properties T10 and T90, and the intercorrelation between natural cetane, aromatics and specific gravity. The correlation matrix also highlights the fact that colinearity between diesel fuel properties is more pronounced than for gasoline, likely due to the fact that gasoline is composed of 7-8 blending streams while diesel fuel is composed of 2-3 streams. For instance, the average of the values in Table I.B-2 (ignoring the diagonal and using the absolute values) is 0.28. By way of comparison, the average correlation coefficient for the fuels used in developing the Complex Model<sup>4</sup> for the reformulated gasoline program was 0.15. Although the selection of fuel properties of interest is somewhat arbitrary in both cases, we can conclude that the degree of colinearity between fuel properties in our diesel emissions database is significantly greater than that in our Complex Model database.

Given the strong colinearities between natural cetane and other fuel properties, it is not surprising that many stakeholders questioned the draft emissions model described in Section I.A. In particular, the NO<sub>x</sub> model contained no natural cetane term, despite the fact that many test programs had shown a strong correlation between natural cetane and NO<sub>x</sub> emissions. On closer examination, the absence of a natural cetane term appears to be a result of "aliasing". The NO<sub>x</sub> model contained both an aromatics and a specific gravity term, and it is likely that these two terms were sufficient to describe the combined effect of aromatics, specific gravity, and natural cetane on NO<sub>x</sub> emissions. The natural cetane effect on NO<sub>x</sub> was, therefore, inherent in the

effects exhibited by aromatics and specific gravity. This concept is supported by the fact that our estimate of NO<sub>x</sub> benefits for the Texas diesel fuel program was the same regardless of whether we used the NO<sub>x</sub> model proposed in our Staff Discussion Document (the model which did not contain a natural cetane term) or an alternative model that contained a total cetane term representing the sum of natural and additized cetane.

The model proposed in our Staff Discussion Document could still be used to predict the NO<sub>x</sub> impacts of changes in natural cetane so long as there existed a means for translating natural cetane changes into the aromatics and specific gravity changes that would likely occur collinearly. Although currently there is no commonly accepted way to do this, we were fortunate in the case of the Texas LED program to have survey data for fuels sold in California. Since Californian diesel fuel was deemed a reasonable representation of fuels that would be produced under the Texas LED program, we could use them to estimate the benefits of the Texas program. The result was that the colinearities between natural cetane and other fuel properties were inherent in the California survey data, and we could place confidence in the resulting predictions from the Staff Discussion Document model.

There exists an alternative way to estimate the impact of changes in cetane number on NO<sub>x</sub> emissions, one that avoids the complication of colinearity between fuel properties. This approach uses additized cetane instead of natural cetane. Additized cetane is largely uncorrelated with other diesel fuel properties, as shown by the low variance inflation factor in Table I.B-1. This result is expected since the additives used to increase cetane generally are used in concentrations of 1 volume percent or less. These low additive concentrations mean that the other components of diesel fuel are not diluted in any measurable way. Also, the properties of the additives themselves are not so extreme that physical properties of diesel fuel such as distillation properties or specific gravity are affected.

There is good reason to believe that additized cetane and natural cetane describe similar, or at least overlapping, combustion mechanisms, since both additized and natural cetane are measures of a fuel's propensity to auto-ignite. Any differences in NO<sub>x</sub> impacts between additized and natural cetane may be related to the aromatics and specific gravity effects that are collinear with natural cetane. That is, natural cetane increases accompanied by typical reductions in aromatics and specific gravity might be expected to produce somewhat larger NO<sub>x</sub> benefits than additized cetane alone. However, we have insufficient information at this time to quantify any potential differences between natural and additized cetane effects on NO<sub>x</sub>.

As a result of our review of colinearities between diesel fuel properties and our current understanding of the impacts of increased cetane number on combustion activity, we have determined that correlating additized cetane number with NO<sub>x</sub> emissions is an appropriate means for providing inventory impact information to States who are considering cetane control programs. The remainder of this technical report describes the analyses we conducted to investigate additized cetane effects on NO<sub>x</sub> emissions.



## II. Analytical approach

### A. Database preparation

The data that we used for our analysis was a subset of the database used to develop the Staff Discussion Document models (discussed in Section I.A). That database was composed of three portions covering engine characteristics, emission measurements, and fuel properties. The fuel properties included values for CETANE\_DIF which represented the increase in cetane number resulting from the addition of a cetane improver additive to conventional diesel fuel. In order to use this database for the analysis of additized cetane effects on NO<sub>x</sub> emissions, we simply deleted (blanked out) any CETANE\_DIF values in the fuel properties database for any test fuels that either did not contain a cetane improver additive, or were not the base fuel to which a cetane improver was added. In the course of curve-fitting using SAS, any fuels with a missing value for CETANE\_DIF were automatically dropped from the analysis. The result was a collection of fuels whose additized cetane values were essentially uncorrelated with other fuel properties. Although the correlation coefficients for additized cetane in Table I.B-2 were low, the data subset used for our analysis produced correlation coefficients that were even lower, as shown in Table II.A-1. A listing of the fuels that were retained for this analysis is given in the Appendix.

Table II.A-1  
Correlation coefficients for additized cetane

	Full database	Subset of database used for additized cetane analysis
Natural Cetane	-0.35	-0.17
Additized cetane	1	1
Sulfur	-0.17	-0.07
Aromatics	0.20	0.01
T10	-0.08	-0.10
T50	-0.07	-0.12
T90	-0.10	-0.10
Specific gravity	0.25	0.04

The final database used in our analysis provided a wide range of measurements for additized cetane and natural cetane number. Figures II.A-1 through II.A-3 show the distribution of cetane values in the database. Note that for Figure II.A-3, none of the base fuels (cetane difference = 0) were included.

Figure II.A-1  
Additized cetane versus natural cetane measurements

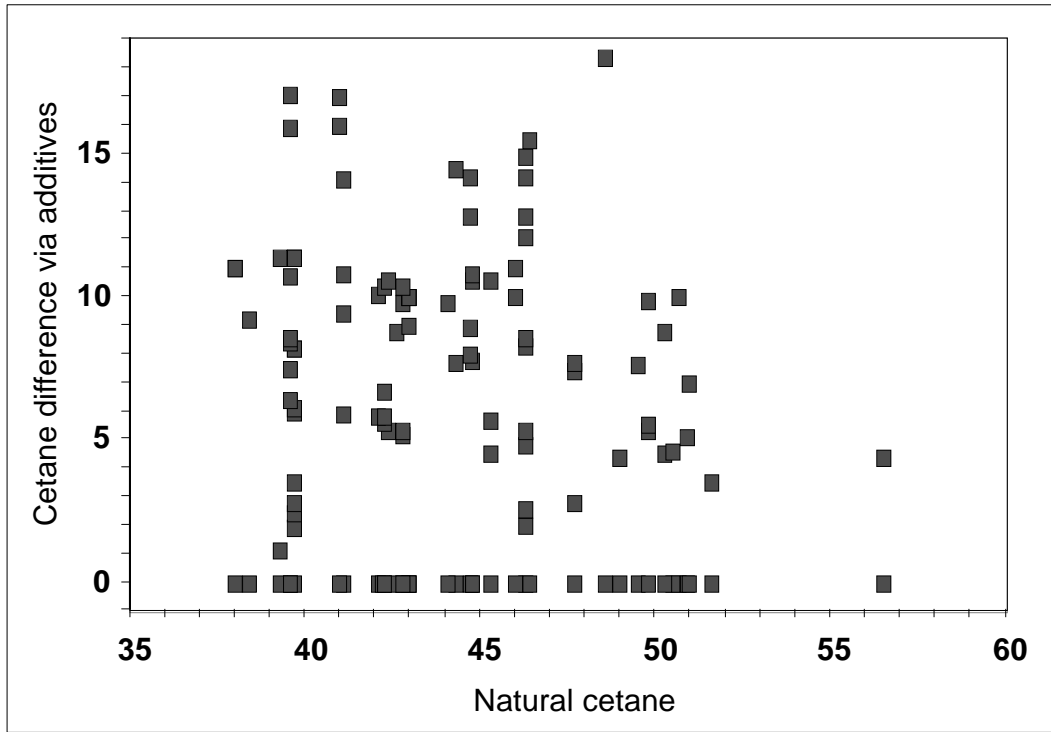


Figure II.A-2  
Natural cetane distribution

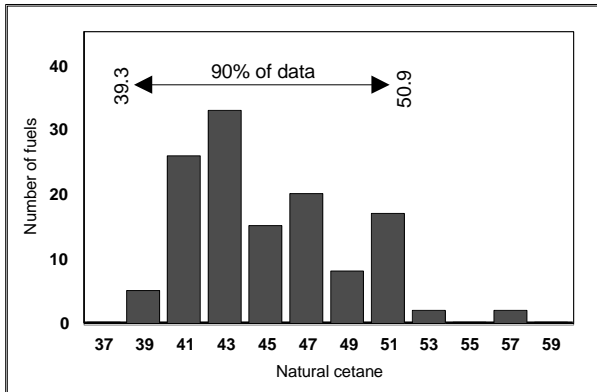
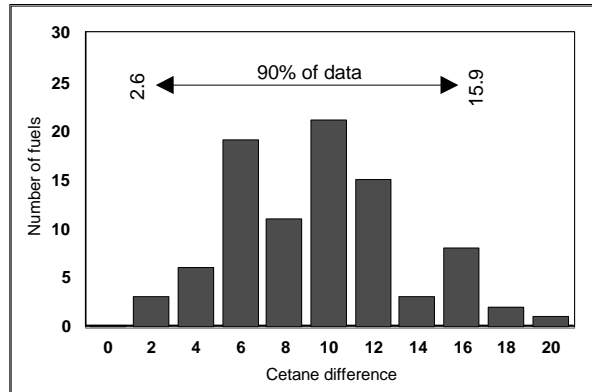


Figure II.A-3  
Additized cetane distribution



Although we eliminated all irrelevant fuels from the fuels dataset, doing so did not guarantee that every engine in the database was tested on both an additized fuel and its corresponding unadditized base fuel. Therefore, we took additional steps to ensure that every engine used in the analysis was tested on both an unadditized fuel and an additized fuel. The result was that all engines from the EPEFE study which received modifications to their injection

timings were excluded. Note that complete descriptions of the full database can be found in the July 2001 Staff Discussion Document.

As in the development of the Staff Discussion Document model, we excluded all data collected on the Japanese 13-mode cycle as being unrepresentative of the federal FTP. We also included all repeat emission measurements (i.e. the same fuel tested on the same engine and cycle multiple times) in the database without averaging those repeats or limiting their inclusion in the database to some maximum number of observations.

## B. Summary of analysis

In correlating additized cetane with NOx emissions, we generally followed the approach described in our July 2001 Staff Discussion Document. This included using the procedure "proc mix" in the statistical analysis package SAS to permit the simultaneous treatment of cetane number as a continuous independent variable and engines as random effects. We chose to use the natural logarithm of NOx emissions to mitigate the heteroscedastic nature of the NOx measurements. We also standardized the independent variables by subtracting the mean and dividing by the standard deviation. The means and standard deviations are shown in Table II.B-1. Standardization removes the scale differences between fuel terms, and also reduces some of the colinearity between first and second-order terms.

Table II.B-1  
Means and standard deviations used for standardizing independent variables

	Mean	Standard deviation
Cetane difference	5.03963	4.94910
Natural cetane	45.13889	4.27954

In our earlier work, we found that technology groups B and L produced different cetane/NOx relationships than other engine technology groups (see Table III.B.3-2 in the Staff Discussion Document). Technology group B represents 2-stroke engines, while technology group L represents engines equipped with exhaust gas recirculation (EGR). For our analysis of additized cetane effects, we chose to exclude all technology group B data. Two-stroke engines currently represent approximately 1 percent of the heavy-duty highway fleet<sup>5</sup>, and are expected to become an even smaller part of the fleet in the future. As a result we do not believe that excluding the group B data from our analysis materially affected the applicability of the results to the in-use fleet.

We also chose to exclude all group L data from our analysis. There are essentially no EGR-equipped engines in the current fleet, but they are expected to become a significant portion of the fleet over the next decade. The Heavy-Duty Engines Workgroup<sup>6</sup> is our primary source for

data on the effects of additized cetane on an EGR-equipped engine, and that data suggests that these engines exhibit no discernable NO<sub>x</sub> response to cetane. Therefore, the NO<sub>x</sub> impacts of additized cetane that resulted from the analyses described below are expected to apply to the entire fleet except EGR-equipped engines, as described more fully in Section III.B.

Engines were identified in *proc\_mix* as categorical random variables in our modeling. This is equivalent to specifying dummy variables for each engine in a fixed model, except that tested engines are treated as a random sample of engines drawn from the full population of engines in the fleet. We also recognized and accounted for two other types of random effects in our modeling. The first is the cetane/NO<sub>x</sub> relationship that is specific to every test engine, and the second is the effect of the unadditized base fuel on NO<sub>x</sub> emissions for each engine. By controlling for these types of random effects, we believe that the overall estimated effect of additized cetane on NO<sub>x</sub> can be confidently applied to the in-use fleet.

The primary independent variable included as a fixed effect in our model was cetane difference, defined as the increase in cetane number brought about through the addition of a cetane improver to conventional diesel fuel. We made no distinction between different types of cetane improver additives since we were not concerned with the effectiveness of a given additive in terms of cetane increase per unit concentration of additive. Instead we treated a given increase in cetane number as having the same effect on NO<sub>x</sub> regardless of the specific additive used to bring about that cetane number increase. This approach is consistent with conclusions reached in several previous studies<sup>7,8,9</sup>. To account for potential nonlinear effects we also included a squared cetane difference term.

Based on past studies of additized cetane effects on emissions, we had some evidence that increases in cetane brought about through the use of additives produced diminishing NO<sub>x</sub> impacts as the base (natural) cetane number of the diesel fuel increased. Thus, for instance, an increase in cetane number from 45 to 50 might be expected to produce larger NO<sub>x</sub> impacts than an increase in cetane number from 50 to 55. To account for this possibility, we introduced a term into the model that represented the interaction of cetane difference and natural cetane number. Figure II.A-1 shows that there is good separation between cetane difference values and natural cetane values, i.e. no correlation exists between the two, which is an important prerequisite for investigating interactive terms. Since the inclusion of an interactive term meant that the natural cetane number was now represented in the model, we decided to also investigate the need for linear and squared natural cetane number terms. The complete list of five terms investigated in this analysis are given in Table II.B-2.

Table II.B-2  
Independent variables investigated  
in correlation between cetane number and NOx

Cetane difference
Cetane difference <sup>2</sup>
Natural cetane
Natural cetane <sup>2</sup>
Cetane difference × natural cetane

Only those terms that were statistically significant at the  $p = 0.05$  level were retained using a backwards stepwise approach. Once all the remaining terms were statistically significant, we identified outliers as any whose residual exceeded four standard deviations from the predicted effect, removed them, and regenerated the model.

### III. Conclusions

#### A. SAS modeling results

The squared natural cetane number term was not statistically significant. After it was dropped and the model regenerated, the remaining terms were all significant. Four outliers were then identified out of 540 total observations. These outliers are listed in Table III.A-1 by the labels used in the database.

Table III.A-1  
Outliers excluded from final model

Study	Engine	Fuel	NOx, g/bhp-hr
SAE902173	902173-1	A3	3.66
SAE902173	902173-1	A3	3.67
SAE902173	902173-1	B2	4.38
SAE902173	902173-1	D1	4.63

Once the outliers were excluded, the model was regenerated a final time. The coefficients for the standardized variables and the associated P-values are given in Table III.A-2.

Table III.A-2  
SAS proc mix output for final model

Variable	Coefficient	P-value
Intercept	1.5060	< 0.0001
Cetane difference	-0.01677	< 0.0001
Cetane difference <sup>2</sup>	0.004139	< 0.0001
Natural cetane	-0.02093	0.0057
Cetane difference × natural cetane	0.004720	< 0.0001

Using the mean and standard deviation for the standardized independent variables (Table II.B-1), we converted the coefficients back into unstandardized form. The fixed effects portion of the resulting model is shown below:

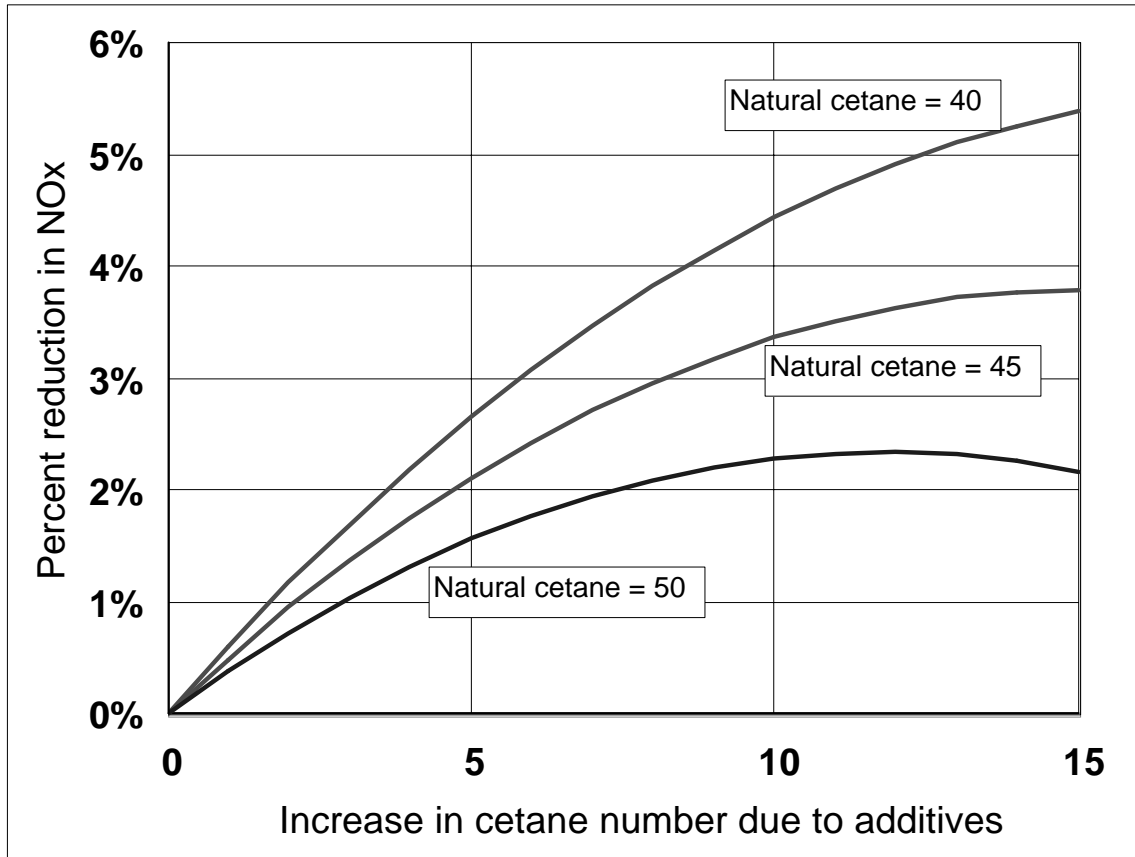
$$\begin{aligned} \ln(\text{NO}_x, \text{g/bhp-hr}) = & 1.79883 & (1) \\ & - 0.015151 \times (\text{cetane difference}) \\ & + 0.000169 \times (\text{cetane difference})^2 \\ & - 0.006014 \times (\text{natural cetane}) \\ & + 0.000223 \times (\text{cetane difference}) \times (\text{natural cetane}) \end{aligned}$$

We can convert this equation into one that provides a percent change in NO<sub>x</sub> emissions as a function of cetane difference and natural cetane. During this conversion, the natural cetane term drops out since natural cetane is the same for the base fuel and the additized fuel. The constant also drops out for the same reason. If the base fuel is assumed to contain no cetane improver additives, the resulting equation is:

$$\begin{aligned} \% \text{ change in NO}_x = & \{ \exp[ - 0.015151 \times (\text{cetane difference}) & (2) \\ & + 0.000169 \times (\text{cetane difference})^2 \\ & + 0.000223 \times (\text{cetane difference}) \times (\text{natural cetane}) ] - 1 \} \times 100\% \end{aligned}$$

The predicted NO<sub>x</sub> impacts are shown graphically in Figure III.A-1.

Figure III.A-1  
 Predicted effect of cetane difference on NOx for all heavy-duty highway engines  
 except 2-strokes and those equipped with EGR



The predicted NOx impact of a given increase in cetane number brought about through the use of additives diminishes as the natural cetane increases, consistent with expectations. However, there are certain conditions under which a "turnover" appears in the predicted effects. For instance, when the natural cetane is 50, the slope of the cetane difference curve changes from positive to negative at a cetane difference of approximately 11.8. We do not believe that these turnovers represent real impacts of additized cetane on NOx emissions, but rather are artifacts of the squared cetane difference term that we used to represent nonlinear effects. We believe it would be appropriate to insert a flat-line extrapolation at the point of any turnover, so that additional increases in cetane number brought about through additives would cause no additional changes in NOx emissions. To do this, we derived a formula that identifies the location of all turnovers as a function of the natural cetane number. This formula is shown below:

$$\text{Turnover in cetane difference} = 44.83 - 0.6598 \times (\text{natural cetane}) \quad (3)$$

Thus for any values of the cetane difference that are larger than the value calculated from equation (3), the predicted NOx impact should be the value calculated from equation (2) using



the cetane difference value calculated using equation (3). In practice, however, we do not believe that this flat-line extrapolation will be necessary. Cetane improver additives are rarely used to increase the cetane number of fuels that already have natural cetane numbers above 55, and even in these cases the additive would have to add more than 8 cetane numbers (for a total cetane number of more than 63) before the turnover would be reached and the extrapolation would be necessary. Far more common is for cetane improver additives to be added to fuels having a natural cetane number in the range of 40 - 50, and then only to raise the total cetane number 5 - 10 numbers. Within these ranges, no turnovers are encountered.

## B. Application to the in-use fleet

As described in Section II.B, we excluded 2-stroke and EGR-equipped engines from our analysis. As a result, equation (2) does not predict NO<sub>x</sub> effects for these types of engines. For 2-stroke engines we do not believe that this result presents a hindrance to the application of equation (2) to the in-use fleet. There were no heavy-duty 2-stroke diesel engines certified for highway use for model years 1998 and 1999, and we expect that this trend will continue in the future. As described in Section II.B, 2-stroke diesel engines currently account for approximately 1% of the heavy-duty highway fleet, so the application of equation (2) to the entire (non-EGR) highway fleet for future years should introduce only negligible error.

Engines equipped with EGR, however, are expected to become an increasingly important part of the highway fleet beginning this year. EGR-equipped engines are expected to exhibit no discernable NO<sub>x</sub> response to cetane. Thus one possible approach to estimating fleet-wide NO<sub>x</sub> effects of cetane improver additives is to use a weighted combination of equation (2), representing engines without EGR, and the zero effect attributable to EGR-equipped engines. Because the relative NO<sub>x</sub> inventories between EGR and non-EGR engines change over time, these weighting factors would be dependent on calendar year.

To estimate these weighting factors, one might use NO<sub>x</sub> inventories that represent the specific areas where the cetane improver additives are intended to be used. For the purposes of generating example weighting factors, we used the nationwide inventory modeling done in the context of our rulemaking setting new standards for heavy-duty engines beginning in 2007 [66 FR 5002]. Using this modeling, we determined how the NO<sub>x</sub> inventory will be distributed among the various model years in the nationwide fleet<sup>10</sup>. We assumed that all 2003 and later heavy-duty diesel engines will have EGR despite the fact that this may be not true for all manufacturers. Lacking a robust means for estimating the fraction of new engine sales that will have EGR in the future, this assumption assures that we are not overestimating NO<sub>x</sub> benefits of cetane control via additives for future years, since EGR-equipped engines have been shown to exhibit no discernable NO<sub>x</sub> response to changes in cetane number. From this information we were able to estimate the fraction of the NO<sub>x</sub> inventory that derived from non-EGR-equipped engines for any calendar year. These fractions are given in Table III.B-1.

Table III.B-1  
Potential yearly weighting factors 'k' for additized cetane model

	Fraction of diesel highway NO <sub>x</sub> inventory which comes from non-EGR-equipped engines
2003	0.93
2004	0.84
2005	0.77
2006	0.70
2007	0.65
2008	0.61
2009	0.57
2010	0.55
2011	0.54
2012	0.53
2013	0.51
2014	0.50
2015	0.48
2016	0.46
2017	0.44
2018	0.41
2019	0.39
2020	0.36

Using the values in Table III.B-1, equation (2) could be modified to represent the entire in-use fleet of heavy-duty diesel highway engines. The result is shown below:

$$\begin{aligned} \text{\% change in NO}_x = & \qquad \qquad \qquad (4) \\ k \times 100\% \times \{ \exp[ & - 0.015151 \times (\text{cetane difference}) \\ & + 0.000169 \times (\text{cetane difference})^2 \\ & + 0.000223 \times (\text{cetane difference}) \times (\text{natural cetane}) ] - 1 \} \end{aligned}$$

There were no nonroad engines in the database we used to evaluate the effects of additized cetane on NO<sub>x</sub> emissions. However, most nonroad engines use technologies similar to those found in highway engines, although in a given year the highway vehicle technology is generally more advanced. Since our previous modeling showed few technology-specific effects of cetane on NO<sub>x</sub>, and even those distinctions have been accounted for in our current analysis by excluding technology groups B and L, any differences between highway and nonroad technology may not be important for additized cetane effects on NO<sub>x</sub>. As a result, it might be appropriate to apply equation (2) to heavy-duty nonroad engines. However, we caution that there exists no robust set of data to validate the use of equation (2) for nonroad, and the concerns we raised in Section VII.B.6 of our Staff Discussion Document regarding this type of extrapolation have not yet been fully addressed.

Finally, we discussed in Section I.B how natural and additized cetane are related, and the fact that additized cetane is more easily analyzed since it can be disassociated from changes in other fuel properties. Based on our current understanding of diesel ignition properties, natural and additized cetane likely represent overlapping effects on combustion and thus on NOx. Although we do not at this time have sufficient information to quantify the differences in NOx effects between natural and additized cetane, preliminary analyses suggest that changes in natural cetane, if accompanied by the collinear changes in aromatics and specific gravity shown in Figure I.B-1, would produce larger NOx benefits than equivalent changes in additized cetane. If so, then equation (4) would provide environmentally conservative predictions of changes in natural cetane. Equation (4) can be modified for application to changes in natural cetane to produce the following:

$$\begin{aligned} \text{\% change in NOx} = & \qquad \qquad \qquad (5) \\ k \times 100\% \times \{ \exp[ & - 0.015151 \times (\text{NATCET}_f - \text{NATCET}_i) \\ & + 0.000169 \times (\text{NATCET}_f - \text{NATCET}_i)^2 \\ & + 0.000223 \times (\text{NATCET}_f - \text{NATCET}_i) \times (\text{NATCET}_i) ] - 1 \} \end{aligned}$$

where

- k = Factor from Table III.B-1 representing engines without EGR
- NATCET<sub>i</sub> = Initial value of natural cetane number
- NATCET<sub>f</sub> = Final value of natural cetane number

### C. Some predicted NOx impacts of additized cetane

The predicted NOx impact of a given change in cetane number is a function of both the calendar year (Table III.B-1) and the natural (or initial) cetane number of the base fuel. We can choose some representative years and base fuel cetane values to predict specific NOx impacts using equations (2) and (4). For instance, one of the primary years in which many current non-attainment areas must show attainment with the ozone standard is 2007. Thus we have made NOx predictions both for the next full calendar year 2003 and for 2007. In this example we also used the current national average cetane number to represent the base fuel for areas that have not implemented a clean diesel fuel program. According to survey data collected by the Alliance of Automobile Manufacturers, the current average cetane number is approximately 45. If we wanted to raise the cetane number of such base fuels to 50, equations (2) and (4) would predict the NOx impacts shown in Table III.C-1.

Table III.C-1  
 Examples of predicted NOx effects (% reduction in NOx)  
 Cetane number increased 5 numbers to 50  
 National average base fuel assumed

	2003	2007
Highway engines	2.0	1.4
Nonroad engines	2.1	2.1

States always have separate NOx inventory estimates for highway and nonroad. We have therefore made no attempt to combine the estimates for highway and nonroad in Table III.C-1 into a single estimate representing total diesel contributions to the NOx inventory.

## Appendix

### Database used in additized cetane analysis

All studies are listed by their database STUDY\_ID label. See Appendix A of Staff Discussion Document for full citations for studies that comprise the full database.

Studies that contained no additized fuels are were therefore eliminated from the additized cetane analysis

ACEA	SAE 852078	SAE 942053
CARB-LOCO	SAE 881173	SAE 961973
CARB-TOXIC	SAE 922214	SAE 961974
SAE 1999-01-1117	SAE 932685	SAE 971635
SAE 1999-01-3606	SAE 932731	SAE 972898
SAE 2000-01-2890	SAE 932734	VE-1_PHASE I
SAE 790490	SAE 932800	

#### Studies/fuels included in the additized cetane analysis

FBATCH_ID	STUDY_ID	CETANE_NUM	CETANE_DIF	BASE FUEL
EPD1	EPEFE	51		
EPD10	EPEFE	58		
EPD11	EPEFE	57.1	7.6	EPD7
EPD2	EPEFE	50.2		
EPD3	EPEFE	50		
EPD4	EPEFE	50.3	0	BASE
EPD5	EPEFE	50.6		
EPD6	EPEFE	50.2		
EPD7	EPEFE	49.5	0	BASE
EPD8	EPEFE	54.8	4.5	EPD4
EPD9	EPEFE	59.1	8.8	EPD4
HDE-10N	HDEWG II	42.3	0	BASE
HDE-11	HDEWG II	48.1	5.8	HDE-10N
HDE-12	HDEWG II	52.7	10.4	HDE-10N
HDE-14N	HDEWG II	42.1	0	BASE
HDE-15	HDEWG II	47.9	5.8	HDE-14N
HDE-16	HDEWG II	52.2	10.1	HDE-14N
HDE-16N	HDEWG II	53.4		
HDE-18	HDEWG II	47.9		
HDE-1N	HDEWG II	42.8	0	BASE
HDE-2	HDEWG II	48	5.2	HDE-1N
HDE-3	HDEWG II	53.2	10.4	HDE-1N
HDE-4N	HDEWG II	42.2	0	BASE
HDE-5	HDEWG II	47.7	5.3	HDE-4N
HDE-6	HDEWG II	53	10.6	HDE-4N
HDE-7N	HDEWG II	42.8	0	BASE

HDE-8	HDEWG II	48.1	5.3	HDE-7N
HDE-8N	HDEWG II	48		
HDE-9	HDEWG II	52.6	9.8	HDE-7N
HDE-R	HDEWG II	46.9		
FUEL1	SAE1999-01-1478	39.7	0	BASE
FUEL1A	SAE1999-01-1478	42.1	2.4	FUEL1
FUEL1B	SAE1999-01-1478	43.2	3.5	FUEL1
FUEL1C	SAE1999-01-1478	45.8	6.1	FUEL1
FUEL1D	SAE1999-01-1478	47.9	8.2	FUEL1
FUEL1E	SAE1999-01-1478	51.1	11.4	FUEL1
FUEL1F	SAE1999-01-1478	41.6	1.9	FUEL1
FUEL1G	SAE1999-01-1478	42.5	2.8	FUEL1
FUEL1H	SAE1999-01-1478	45.7	6	FUEL1
FUEL1I	SAE1999-01-1478	47.9	8.2	FUEL1
FUEL1J	SAE1999-01-1478	51.1	11.4	FUEL1
FUEL2	SAE1999-01-1478	46.3	0	BASE
FUEL2A	SAE1999-01-1478	48.9	2.6	FUEL2
FUEL2B	SAE1999-01-1478	51.6	5.3	FUEL2
FUEL2C	SAE1999-01-1478	54.6	8.3	FUEL2
FUEL2D	SAE1999-01-1478	59.1	12.8	FUEL2
FUEL2E	SAE1999-01-1478	60.5	14.2	FUEL2
FUEL2F	SAE1999-01-1478	48.3	2	FUEL2
FUEL2G	SAE1999-01-1478	51.1	4.8	FUEL2
FUEL2H	SAE1999-01-1478	54.9	8.6	FUEL2
FUEL2I	SAE1999-01-1478	58.4	12.1	FUEL2
FUEL2J	SAE1999-01-1478	61.2	14.9	FUEL2
0	SAE902172	42.5		
1	SAE902172	39.9		
2	SAE902172	39.6	0	BASE
2A	SAE902172	47.1	7.5	2
2B	SAE902172	55.5	15.9	2
2S	SAE902172	39.6		
4	SAE902172	46.4	0	BASE
4B	SAE902172	61.9	15.5	4
5	SAE902172	48.6	0	BASE
5B	SAE902172	67	18.4	5
6	SAE902172	51.8		
A1	SAE902173	45.3	0	BASE
A2	SAE902173	49.8	4.5	A1
A3	SAE902173	51	5.7	A1
A4	SAE902173	55.9	10.6	A1
B1	SAE902173	39.6	0	BASE
B2	SAE902173	46	6.4	B1
B3	SAE902173	48	8.4	B1
B4	SAE902173	48.2	8.6	B1
B5	SAE902173	50.3	10.7	B1
B6	SAE902173	56.7	17.1	B1

C1	SAE902173	47.7	0	BASE
C2	SAE902173	50.5	2.8	C1
C3	SAE902173	55.1	7.4	C1
C4	SAE902173	55.4	7.7	C1
D1	SAE902173	49.8	0	BASE
D2	SAE902173	55.1	5.3	D1
D3	SAE902173	55.3	5.5	D1
D4	SAE902173	59.7	9.9	D1
C1	SAE910735	42		
C2	SAE910735	44.8	0	BASE
C2I	SAE910735	52.6	7.8	C2
C2S	SAE910735	43.8		
CR	SAE910735	50.8		
DD10	SAE912425	62.7		
DD11	SAE912425	53.1		
DD12	SAE912425	47		
DD4	SAE912425	50.7	0	BASE
DD5	SAE912425	60.7	10	DD4
DD8	SAE912425	50.2		
DD9	SAE912425	50.7		
A	SAE922267	51.6	0	BASE
B	SAE922267	55.1	3.5	A
C	SAE922267	54.6		
D	SAE922267	42.3	0	BASE
E	SAE922267	47.9	5.6	D
F	SAE922267	49	6.7	D
G	SAE922267	38.4	0	BASE
H	SAE922267	47.6	9.2	G
I	SAE922267	47.3		
J	SAE922267	52		
K	SAE922267	39.6		
L	SAE922267	50.4		
LS	SAE932767	43	0	BASE
LS-N	SAE932767	52	9	LS
LS-P	SAE932767	53	10	LS
A	SAE942019	46	0	BASE
A-DTBP	SAE942019	57	11	A
A-EHN	SAE942019	56	10	A
B	SAE942019	41	0	BASE
B-DTBP	SAE942019	58	17	B
B-EHN	SAE942019	57	16	B
C	SAE942019	38	0	BASE
C-DTBP	SAE942019	49	11	C
C-EHN	SAE942019	49	11	C
D	SAE942019	43	0	BASE
D-EHN	SAE942019	53	10	D
D-EHN/DTBP	SAE942019	53	10	D

A-1	SAE970758	56		
A-10	SAE970758	53	10	A-9
A-2	SAE970758	65		
A-3	SAE970758	43		
A-4	SAE970758	60		
A-5	SAE970758	58		
A-6	SAE970758	56		
A-7	SAE970758	51	0	BASE
A-8	SAE970758	58	7	A-7
A-9	SAE970758	43	0	BASE
MAN18	SAE972894	58.7		
MAN2	SAE972894	50.9	0	BASE
MAN2*	SAE972894	56	5.1	MAN2
MAN7	SAE972894	56.5	0	BASE
MAN7*	SAE972894	60.9	4.4	MAN7
A	SAE972904	44.8	0	BASE
B	SAE972904	50.5	0	BASE
C	SAE972904	54.7		
D	SAE972904	55.4	10.6	A
E	SAE972904	55.6	10.8	A
F	SAE972904	55.1	4.6	B
VE 10 A	VE 10	44.3	0	BASE
VE 10 AA	VE 10	41.1	0	BASE
VE 10 B	VE 10	52	7.7	VE 10 A
VE 10 BB	VE 10	47	5.9	VE 10 AA
VE 10 C	VE 10	58.8	14.5	VE 10 A
VE 10 CC	VE 10	50.5	9.4	VE 10 AA
VE 10 D	VE 10	50.8		
VE 10 DD	VE 10	51.9	10.8	VE 10 AA
VE 10 E	VE 10	51.5		
VE 10 EE	VE 10	55.2	14.1	VE 10 AA
VE 10 F	VE 10	51.4		
VE 10 FF	VE 10	44.7	0	BASE
VE 10 G	VE 10	50.5		
VE 10 GG	VE 10	52.7	8	VE 10 FF
VE 10 H	VE 10	54.2		
VE 10 HH	VE 10	53.6	8.9	VE 10 FF
VE 10 I	VE 10	59.4		
VE 10 II	VE 10	57.5	12.8	VE 10 FF
VE 10 J	VE 10	46.3		
VE 10 JJ	VE 10	58.9	14.2	VE 10 FF
VE 10 K	VE 10	54.3		
VE 10 KK	VE 10	51.7		
VE 10 L	VE 10	54.3		
VE-1A	VE-1_PHASE II	42.6	0	BASE
VE-1B	VE-1_PHASE II	51.4	8.8	VE-1A
VE-1C	VE-1_PHASE II	55.1		



VE-1D	VE-1_PHASE II	39.3	0	BASE
VE-1E	VE-1_PHASE II	40.4	1.1	VE-1D
VE-1F	VE-1_PHASE II	50.7	11.4	VE-1D
VE-1G	VE-1_PHASE II	49	0	BASE
VE-1H	VE-1_PHASE II	53.4	4.4	VE-1G
VE-1K	VE-1_PHASE II	44.1	0	BASE
VE-1L	VE-1_PHASE II	53.9	9.8	VE-1K
VE-1M	VE-1_PHASE II	48.6		
VE-1N	VE-1_PHASE II	38.5		
VE-1O	VE-1_PHASE II	49.2		

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