REPORT REVIEW

EPA420-S-02-012 – THE EFFECT OF CETANE NUMBER INCREASE DUE TO ADDITIVES ON NOX EMISSIONS FROM HEAVY-DUTY HIGHWAY ENGINES

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

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INTRODUCTION

The U. S. Environmental Protection Agency (EPA) requested an independent peer review of the report entitled “The Effect of Cetane Number Increase Due to Additives on NOx Emissions from Heavy-Duty Highway Engines.” This report, numbered EPA420-S-02-012, is dated June 2002 and is labeled as a revised draft technical report. EPA believes that the analysis presented in the report is an “appropriate means” for calculating the impacts of higher cetane diesel fuel on NOx emissions.

The letter requesting the review[1] asked that the following questions be addressed.

1. Is the range of fuels and engines in the database sufficient to form the basis of estimated effects of additized cetane on NOx emissions for the in-use fleet?
2. Is it reasonable to conclude that additized cetane effects on NOx are independent of engine model year?
3. Is it reasonable to assume that all engines sold after 2002 will make use of exhaust gas recirculation?
4. Is there reasonable agreement between the data and the model?

The overall directions for review also call for a clear distinction “between recommendations that are necessary to ensure the adequacy of the predictions and those that [. . .] should be considered but are not critical.”

The body of this review is in the next section. That discussion section presents a brief overview of the report and some general comments. It then addresses the four questions listed above. Finally, additional comments, some simply editorial, are made regarding the report. The recommendations section summarizes the comments and distinguishes between essential recommendations and those that are not critical.

The report draft provided for review was an intermediate draft in which a blank page with the heading “I. EPA Technical Reports” was inserted as a placeholder for material to be added later. Although the remaining sections of the report were renumbered to be consistent with this new section, the tables and figures were not. The discussion in this review of specific report sections, figures, and tables uses the numbers in the draft even though they are not consistent.

[1]Chester L. France letter to Larry Caretto, August 22, 2002.

DISCUSSION

Scope of the report

The EPA report provides a statistical analysis of existing data on the emission effects of two variables in fuel used in on-highway heavy-duty diesel engines: natural cetane and additized cetane. The latter is defined as the increase in cetane produced by diesel fuel additives designed to increase cetane number.

This report is the result of a process that started in fall 2000 when "EPA voiced concern about the NOx emission reduction credits claimed by Texas [for its low emission diesel (LED) program]." Prior to this report there were meetings with "numerous stakeholders," a July 2001 contractor report by Southwest Research Institute (SwRI),[2] and a July 2001 EPA staff discussion document by EPA.[3] There was also a public workshop held on August 28, 2001. EPA established a web site[4] for this issue that has various reports and memoranda related to this study and stakeholder comments from the public meeting.

The introduction to the report notes that EPA's conclusions on the Texas program were transmitted in a separate memo. It further states that "there is 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."

General Comments

In a study like this one, it would be useful to have some quantitative measure of the uncertainty in the results, such as the final regression equation plotted in Figure III.B.1 on page 21. Regression equations by other researchers are shown on the same plot indicating a wide spread in the work of various groups. On this graph it appears that an increase of five in the cetane number due to additives will reduce NOx by about 2% using the regression equation proposed here. However, the other regression equations

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[2] Robert L. Mason and Janet P. Buckingham, "Diesel Fuel Impact Model Data Analysis Plan Review, Draft Final Report, Work Assignment 2-7, EPA Contract 68-C-98-169, Southwest Research Institute, July, 2001.

[3] U. S. Environmental Protection Agency, Strategies and Issues in Correlating Diesel Fuel Properties with Emissions, Staff Discussion Document EPA420-P-01-001, July 2001.

[4] http://www.epa.gov/otaq/models/analysis.htm

shown in the figure predict a NOx reduction in the range of 1% to 3% for the same increase in cetane number. Showing the confidence limits on this regression would give the reader some indication of the reliability of the equation for making predictions. Other areas where confidence limits would add to the report are noted below.

Is the range of fuels and engines in the database sufficient to form the basis of estimated effects of additized cetane on NOx emissions for the in-use fleet?

Fuels

There are two separate questions one can ask regarding the fuels. The question asked here regards the range of fuels. This is separate from the representativeness of the fuels that is addressed in section III.A-1 of the report.

The data to respond to both issues – range and representativeness – are shown in Figures II.A-1 and II.A.1-1 to II.A.1-6 of the report. Figure II.A.1-1 shows a wide range for the natural cetane and cetane differences in the database fuels. This figure shows that the range of values for these properties, which are the ones used in the regressions derived in the report ,are sufficiently broad to form the basis for the resulting regressions.

The issue of representativeness is less certain. Because of the small effect of fuels on emissions (compared to engine effects) and the correlations among various fuel properties, studies of fuel effects on emissions use specially chosen fuels. Such fuels have a wide range in properties to enable effects to be determined with a reasonable number of experimental measurements. In addition, these fuels are often custom blended to avoid collinear effects. This results in experimental fuels that are somewhat different from in-use fuels. This is shown in Figures II.A.1-1 to II.A.1-6 of the report. The distribution of fuel properties, especially sulfur, aromatics, specific gravity and T90, is much narrower in the in-use survey data than it is in the fuels used in the database. Only natural cetane has a similar distribution in both cases.

The report compares the fuel property distributions from the survey data and the report database in terms of the ranges that encompass 90% of the data. This comparison leads the report authors to the conclusion on page 12 that the "database is fully representative of in-use fuels." This conclusion is correct for the range of properties, but not for the distribution. A more appropriate conclusion is that the fuels in the database have been selected for experimental studies of fuel effects on emissions. Although there are differences in the distribution of properties when the database fuels are compared to in-use surveys, the range of the fuels is the same and there should be no significant differences in the additized cetane response for the two sets of fuels.

Engines

The representativeness of the engines used in the report is analyzed in section III.A.2 in terms of the model year distribution. Twenty-two engines were present in the database with the following model-year distribution: 1991 (5), 1993 (4), 1994 (7), 1996 (5), and 1998 (1). Although the report notes that two-stroke engines and engines with exhaust gas recirculation (EGR) were excluded from the database, there is no analysis of the technology groups to which the remaining engines belong.

Table II.C-2 in the staff discussion document[3] lists of the number of engines and the relative amount of emission data in the various technology groups in the original database. The table shows 73 engines in 16 technology groups in the original database.[5] The technology groups in the original database represent a wide range of in-use engines. Technology groups F and T[6] account for 60% of the emissions data in the original database. When the data for two-stroke engines and EGR-equipped engines are eliminated, there are 65 engines in the original database and groups F and T account for 64% of the emissions data there.

The database-preparation discussion in section III.A of the report refers to the staff discussion document for information about the basic database. The database-preparation procedures were presumably responsible for reducing the number of engines from 73 in the original database to 22 used in this study.

The data on engines built during the 1990s should be representative of the onroad national fleet. In addition, since the proposed final equation allows no credit for engines produced in 2003 and later, the model year mix used for the engines that receive cetane credit will not change significantly as new engines are introduced into the fleet. On this basis, the engines used in the database should be representative.

Because there is no analysis in the report that compares the technology groups of the engines in the database with the engines in the fleet, it is not possible to answer the question of whether or not the range of engines in the database is sufficient. Such an

[5] The text that references this table states that there were 75 engines (some of which were the same engine with different injection timings) in 17 technology groups. The discussion here is based on the data actually in the table.

[6] Both of these technology groups represent turbocharged, direct-injection engines. Group F uses mechanical (inline or rotary) fuel injection and has displacements less than or equal to 9.4 L.. Group T uses electronic unit injection and has displacements greater than 9.4 L.

analysis would give a better picture of the similarities and differences between the onroad fleet and the fleet in the database.

On page 23, the report notes that one might use local inventory data on fleet distribution. Urban areas are expected to have a larger proportion of older engines than the national fleet. The regression equation in this report should also be applicable to these areas with the different fleet distributions.

Is it reasonable to conclude that additized cetane effects on NOx are independent of engine model year?

The report contains an analysis in which the effect of a unit increase in cetane on NOx reduction was analyzed as a function of model year. The data for this analysis are plotted in Figure II.A.2.2 on page 14 of the report. According to the discussion on that page, two separate analyses – one accounting for an engine effect and one without such an effect – showed no statistically significant slope at the $p = 0.1$ level.

This analysis supports the conclusion that the additized cetane effects are independent of model year. However it would be interesting to learn the slope of the regression slope and its p-value.

Is it reasonable to assume that all engines sold after 2002 will make use of exhaust gas recirculation?

The significance of this question is related to the application of the proposed model to the future in-use fleet. The report proposes, in the discussion that begins at the bottom of page 22, that there is no NOx reduction credit for cetane increase in 2003-and-later engines. The absence of cetane effect on 2003-and-later engines is attributed to the presence of EGR on these engines. Because it is not intuitively obvious why EGR should negate the effect of cetane, this review examined the basis for the conclusion about EGR effects.

New emission control technologies are likely to be required to meet the diesel emission standards for 2004. Those standards lower the allowed non-methane hydrocarbons (NMHC) from 1.2 to 0.5 g/bhp-hr, and the current NOx standard of 4 g/bhp-hr will be cut approximately in half.[7] These emission reductions on the diesel engines that have

[7] There is no actual NOx standard for 2004. Instead, the engine manufacturers must meet a combined NMHC + NOx standard of 2.4 g/bhp-hr; manufacturers can choose to meet an optional NMHC + NOx standard of 2.5 g/bhp-hr combined with a NMHC standard of 0.5 g/bhp-hr.

already been subject to significant control will require new control technologies of which exhaust gas recirculation (EGR) is the most likely candidate. The even more stringent diesel emission standards for 2007 will almost certainly require add-on controls for NOx and particulate matter (PM) standards; however, the 2007 standards will continue to require control in the engine itself in addition to the add-on controls.

Under the terms of a 1998 settlement to a civil suit, seven engine manufacturers, who produce nearly all the heavy-duty diesel engines sold in the U. S., agreed to implement the 2004 standards for all engines sold on or after October 1, 2002. Thus, the emission control technology anticipated for the 2004 standards will be on virtually all heavy-duty diesel engines starting from this October 2002 date. The report uses 2003 and later as the starting point for the installation of technology that meets the new standards.

EPA's relationship with manufacturers regarding future certification plans should give them more data about specific manufacturer's plans regarding future emission control technology than is available to this reviewer. On page 13, the report notes that "there are indications that some manufacturers will not use EGR in their 2002+ engines." Although no quantitative data are presented, there is an implication that the majority of new engines will be using EGR.

Page 15 of the report cites a report by the Heavy-Duty Engines Workgroup (HDEWG) as the "primary source for [EPA's] data on the effects of additized cetane on an EGR-equipped engine." The results from the HDEWG were published in a series of SAE papers in 2000. One paper, which presented the statistical analysis of the study,[8] had the following observations about the effect of cetane:

1. The overall conclusion was that the engine had a "very low sensitivity to cetane number . . . [that] differs from the results of similar experiments in engines that are not equipped with EGR."
2. Table 5 of the paper showed that the regression coefficient for NOx with cetane had a small positive value whose p-value (level of significance) was 0.024.
3. Figure 2 showed that an increase in cetane number from 42 to 52 would *increase* NOx by 1.3%.

The paper reported data with and without EGR, but did not explicitly compare the effects of cetane on NOx, with and without EGR. Table 1, below, is taken from Table 8 of the statistical results paper.[8] The NOx results in this table are the averages of the

[8] Robert L. Mason *et al*. "EPA HDEWG Program – Statistical Analysis," SAE Paper 2000-01-1859, presented at International Spring Fuel and Lubricants Meeting, Paris, France, June 19-22, 2000.

entries for two fuels with the same cetane number in the original paper. The fuels that have an N in their designation are natural cetane fuels that do not have any additized cetane. *E.g*., fuels 16 and 16N are both reported as having a “target” cetane level of 52. (The paper contained an analysis that showed the effect of cetane was the same whether the cetane number was produced by an additive or by natural cetane.)

Table 1 – HDEWG Data for Cetane NOx Effect With and Without EGR[8]

Fuels	Cetane	NOx data with EGR			NOx without EGR		
		g/bhp-hr	Percent change		g/bhp-hr	Percent change	
7N+14N	42	2.368	Per step	Initial to final	3.740	Per step	Initial to final
8+8N	47	2.415	2.0%		3.803	1.7%	
16+16N	52	2.346	-2.9%	-0.9%	3.684	-3.1%	-1.5%

The results of Table 1 show that the effect of cetane on NOx is similar with or without EGR, for the engine used in the study. In both cases there is an increase of about 2% as the cetane number is increased from 42 to 47 and a decrease of about 3% as the cetane number is increased from 47 to 52. The overall effect of increasing the cetane number from 42 to 52 is a NOx decrease of 0.9% with EGR and a NOx decrease of 1.5% without EGR.

This table shows that the effects of cetane on NOx for this engine are similar with and without EGR. Although the engine has a low sensitivity to cetane, it is likely that this effect is not due to EGR. Instead, it is due to some other differences between this engine and engines tested previously.

One possible explanation may be found in the paper that presents the HDEWG engine test results.[9] Figures 9 to 12 of that paper, and the discussion of those figures, notes that “there is very little premixed burning.” Since the premixed burning phase of diesel combustion is the one that is affected by changes in cetane number, an engine that is designed to nearly eliminate this premixed-burning phase should have a low sensitivity to cetane. The report notes (on page 13) that EPA has “limited information” suggesting that this hypothesis is correct.

[9] Andrew C. Matheaus, *et al*. “EPA HDEWG Program – Engine Tests Results,” SAE Paper 2000-01-1858 presented at International Spring Fuel and Lubricants Meeting, Paris, France, June 19-22, 2000.

According to the full database that EPA used for this study,[10] all the EGR engine data (technology group L) are taken with a single engine, a Caterpillar 3176. Thus the conclusion that cetane has no effect on EGR-equipped engines is not supported by tests on different engines.

This section is supposed to address the following question: is it reasonable to assume that all engines sold after 2002 will make use of exhaust gas recirculation? This question is better restated: Is it reasonable to assume that engines calibrated to meet emission requirements for engines manufactured in 2003-and-later will be designed so that cetane has no effect on NOx emissions?

The answer to the revised question is a guarded "yes." The only data available for fuel effects on such an engine indicate that cetane will not have a sizeable effect on NOx. (Furthermore the effect of cetane in the one engine tested is a slight – but statistically significant – *increase* in NOx.) A review of the SAE papers discussing the tests on this engine suggests that the explanation for this effect may be the control of the combustion process to reduce premixed burning rather than EGR. However, this proposed explanation does not change the conclusion of the report that no NOx reduction credit should be given for cetane use in highway engines designed to meet the "2004" emission standards.

The conclusion could be less guarded if data were available in more than one engine designed to meet these standards. However, there are no data that conflict with the observations that one engine calibrated to meet the 2004 emission standards shows a small effect of cetane on NOx emissions and that effect is an increase NOx.

Is there reasonable agreement between the data and the model?

The p-values for the significance of the regression coefficients, shown in Table III.A-2 are all less than 0.0001 except for the natural cetane coefficient which is 0.0057; these small p values show a good fit of the model to the data.

Figure II.B-2 on page 22 shows a comparison of predicted versus observed NOx changes. This plot shows a significant scatter around the 45^o line on which all data should ideally fall. Most of the individual data points lay in a band that is ±2.5 percentage points on either side of the 45^o line. The wide scatter of individual data points around the 45^o line is typical of such plots when examining the effects of fuels on emissions. It would be interesting to know the confidence limits for the mean observed

[10]This was taken from the Excel file hdd-db7.xls, available at the EPA diesel analysis web site, http://www.epa.gov/otaq/models/analysis.htm.

change. The report notes that a regression line through these data had “a slope that is close to 1.0.” The confidence limits on the mean for this regression line would give a quantitative estimate of the agreement between the data and the model.

Although it would be helpful to have the quantitative confidence limit recommended in the previous paragraph, the low p-values for the regression coefficients and the visual comparison of the observed and predicted data in Figure III.B-2 show reasonable agreement between the data and the model.

Other comments

The suggestion on page 25 that a modified version of equation (4) could be applied to changes in natural cetane is not consistent with the equations previously derived. Equation (4) is derived from the percent reduction equation (2). Equation (2) is derived from the basic regression equation (1) by assuming that the percent reduction is due only to additized cetane. The natural cetane of the base fuel and the additized fuel are assumed to be the same. Accordingly, the natural cetane number term drops out of equation (2). If equation (2) were written to consider changes in both additized cetane and natural cetane it would be written as follows.

$$\begin{aligned}\text{fractional change in NOx} = \exp\{ & -0.015151\,[\,cetDiff_f - cetDiff_i\,] \\ & + 0.000169\,[\,cetDiff_f - cetDiff_i\,]^2 \\ & - 0.006014\,[\,natCet_f - natCet_i\,] \\ & + 0.000223\,[\,(natCet_f)(cetDif_f) - (natCet_i)(cetDif_i)\,] - 1\,\}\end{aligned}$$

In this equation $natCet_i$ and $natCet_f$ represent the initial natural cetane number of the initial (base) fuel and $natCet_f$ represents the natural cetane number of the final (modified) fuel. Similarly $cetDiff_i$ and $cdtDiff_f$ represent the cetane difference due to additives in the base fuel and the modified fuel, respectively. Equation (5) substitutes the natural cetane terms for the additized cetane terms and does not consider any possible changes in cetane additives between the base and modified fuel.

The discussion of equation (5) implies that the additized cetane equation may be used to estimate, for regulatory purposes, the effects of changes in natural cetane. No reason is given in that discussion for not providing an equation that specifically considers the effects of natural cetane on NOx. Presumably, this was due to the problems associated with modeling natural cetane because of its correlations with other fuel properties. The report should discuss any alternatives to equation (5) that were considered and rejected.

The report could benefit from a brief abstract stating the purpose of the report and the overall conclusions. At present one gets to the bottom of page six before learning that

EPA has “determined that correlating of additized cetane with NOx is an appropriate means for providing inventory impact information to anyone considering the use of higher cetane diesel fuel.”

The conclusion near the bottom of page 24 that it “might be appropriate to apply” the regression equation to nonroad engines is not very definitive. Should an area planning a diesel fuel control program claim credit for NOx reductions from nonroad engines? If no policy decision on this issue has been made, the report should say so explicitly. Of course, there are no data on cetane effects in nonroad engines, but one would expect that the NOx effects in nonroad and onroad engines to be similar. A given percent reduction in NOx emissions could become a more significant emission reduction in nonroad engines due to the higher emission rates and longer lifetimes for these engines as compared to highway engines.

Minor editorial comments

The numbering of tables and figures (and the references to these) needs to be redone to reflect the addition of a new section I, EPA Technical Reports. (This section has only its title and a note that the section will be included in the final report.) There are also references to sections that will have to be corrected; *e.g.*, the reference in the next-to-last line on page 12 should be “Section III.B” instead of II.B.

The equation defining the variance inflation factor should be placed in the final paragraph of page 3 where this term is introduced.

The reference for the data in Figure 1.B-1 on page 3 is a 1999 AAM fuel survey. It would be helpful to the reader to indicate briefly in the text, at the point where the reference is made, that the data in the figure come from an in-use survey. This would make it clear that the Figure 1.B-1 and Table 1.B-1 are based on the same data set. At present the mention of in-use survey data, at the top of page 4, is not clear. In addition there is presently a reference to AAM data collected in 2000 on page 9 of the report. Is this a different survey or the same one as cited earlier?

It would be helpful to modify the bar chart in Figure II.A.2-1 on page 13 so that the number of engines for each model year is shown at the top of the bars.

No mention is made of the EPA diesel fuel analysis web site in the report. This is a useful site for anyone who wants to review the background for the present report. This site could be mentioned in the introduction or as a preface to the references section.

The word calendar is misspelled[11] at various places in the report: page 23, last line in both second and third paragraph; page 25, last paragraph, second and sixth lines.

[11]The spelling used in the report, calender, is allowed by the spell checker in Word Perfect. According to www.dictionary.com, a calender is “a machine in which paper or cloth is made smooth and glossy by being pressed through rollers.” This misspelling may be in other places in the report not listed above.

RECOMMENDATIONS

Recommendations necessary to ensure the adequacy of the predictions

The comments in the previous section deal mainly with editorial changes and recommendations for inclusion of more statistical information about existing results. Based on this review there appears no problem with the immediate use of the equations in the report to make useful estimates of the NOx reductions due to the addition of cetane improvers to diesel fuel.

If there is significant use of this approach in future years, the database that justifies the assumption that engines built in 2003-and-later will have no NOx benefit from cetane addition should be based on a larger set of engine data.

Recommendations that should be considered but are not critical

The various recommendations that were made in the previous section are not critical to ensure the adequacy of the predictions. However, these recommendations, summarized below, could improve the usefulness of the report.

- Compare the distribution of engine technology groups in the database with those in the in-use fleet to determine how well the range of engines tested matches those in use.
- Include confidence limits for the final regression equation and the prediction of measured and predicted data.
- Review evidence for cause of low cetane sensitivity in engines equipped with EGR. If you agree that the lack of a cetane effect is not just due to EGR, but to other advanced emission control systems, revise the report accordingly.
- Consider a future test program to verify cetane effects on advanced emission control systems, if cetane increases become a significant NOx control strategy.
- Describe any alternatives to equation (5) that were considered to model the effects of natural cetane changes on NOx.
- Clarify the policy guidance on the application of this analysis to nonroad engines.