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Energy Division

**REFORMULATED GASOLINE:
COSTS AND REFINERY IMPACTS**

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ACRONYMS AND ABBREVIATIONS

ACCA	Advanced Computing Center of Argenta
API	American Petroleum Institute
ASTM	American Society for Testing and Materials
BTX	Benzene, toluene, and xylenes
CAAA	Clean Air Act Amendments of 1990
CG	Conventional gasoline
CO	Carbon monoxide
DCF	Discounted cash flow
DOE	Department of Energy
EIA	Energy Information Administration
EPA	Environmental Protection Agency
ETBE	Ethyl tertiary butyl ether
F	Fahrenheit
FCC	Fluid catalytic cracker
gal	Gallon
gm/mi	Grams per mile
MBD	Thousand barrels per day
mg/mi	Milligrams per mile
MMSCFPSD	Million standard cubic feet per stream day
MTBE	Methyl tertiary butyl ether
NMHC	Nonmethane hydrocarbon
NOX	Nitrogen oxides
NPC	National Petroleum Council

NPRA	National Petroleum Refiners Association
ORNL	Oak Ridge National Laboratory
ORNL-RYM	Oak Ridge National Laboratory Refinery Yield Model
PADD	Petroleum Administration for Defense District
ppm	Parts per million
psi	Pounds per square inch, absolute
Reg-Neg	Negotiated rule making
REMS	Refinery Evaluation Modeling System
RFG	Reformulated gasoline
ROI	Return on investment
RVP	Reid vapor pressure
SIP	State Implementation Plan
TAAE	Tertiary amyl ethyl ether
TAME	Tertiary amyl methyl ether
TAP	Toxic air pollutant
THEE	Tertiary hexyl ethyl ether
THME	Tertiary hexyl methyl ether
TMC	Turner, Mason & Company
T50	The temperature at which 50 percent of a fuel is evaporated in ASTM test D86-67: Distillation of Petroleum Products
T90	The temperature at which 90 percent of a fuel is evaporated in ASTM test D86-67: Distillation of Petroleum Products
VOC	Volatile organic compound
vol	Volume
wt	Weight

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ABSTRACT

Studies of reformulated gasoline (RFG) costs and refinery impacts have been performed with the Oak Ridge National Laboratory Refinery Yield Model (ORNL-RYM), a linear program which has been updated to blend gasolines to satisfy emissions constraints defined by preliminary complex emissions models. Policy makers may use the reformulation cost knee (the point at which costs start to rise sharply for incremental emissions control) to set emissions reduction targets, giving due consideration to the differences between model representations and actual refining operations. ORNL-RYM estimates that the reformulation cost knee for the U.S. East Coast (PADD I) is about 15.2 cents per gallon with a 30 percent reduction of volatile organic compounds (VOCs). The estimated cost knee for the U.S. Gulf Coast (PADD III) is about 5.5 cents per gallon with a VOC reduction of 35 percent. Reid vapor pressure (RVP) reduction is the dominant VOC reduction mechanism. Even with anti-dumping constraints, conventional gasoline appears to be an important sink which permits RFG to be blended with lower aromatics and sulfur contents in PADD III. In addition to the potentially large sensitivity of RFG production to different emissions models, RFG production is sensitive to the non-exhaust VOC share assumption for a particular VOC model. ORNL-RYM has also been used to estimate the sensitivity of RFG production to the cost of capital; to the RVP requirements for conventional gasoline; and to the percentage of RFG produced in a refining region.

REFORMULATED GASOLINE: COSTS AND REFINERY IMPACTS

EXECUTIVE SUMMARY

The Clean Air Act Amendments of 1990 (CAAA) will have far-reaching effects on the refining industry because, in addition to complying with all other CAAA provisions, refiners will have to modify, design, permit, and construct new units to produce mandated cleaner products such as reformulated gasolines (RFGs).

For RFGs, the law specifies a minimum oxygen content; a maximum benzene content; maximum summer Reid vapor pressures (RVPs); no heavy metals; no increase in nitrogen oxide (NOX) emissions; and reductions in emissions of ozone-forming volatile organic compounds (VOCs) and toxic air pollutants, relative to established baselines.

The CAAA requires a formal fuel certification procedure for demonstrating the emissions performance of a gasoline. Emissions modeling provides a means for predicting the emissions performance of a gasoline, given other physical and chemical properties of the gasoline.

The Complex Model will be a set of equations that predicts emissions in terms of the values of a number of gasoline properties. A preliminary Complex Model published by the Environmental Protection Agency (EPA) in October 1992 included the gasoline properties of RVP, T50, T90, benzene, oxygen, sulfur, aromatics, and olefins contents.

Studies of RFG costs and refinery impacts have been performed with the Oak Ridge National Laboratory Refinery Yield Model (ORNL-RYM), a linear program which has been updated to blend gasolines to satisfy emissions constraints defined by preliminary complex emissions models. Non-linear emissions models of the Department of Energy (DOE) and EPA have been represented in ORNL-RYM by assuming that an emission value can be represented as a base emission value plus small linear emissions changes due to small changes in gasoline properties.

The updated ORNL-RYM has been used to estimate costs and refining impacts for producing RFGs in the U.S. East Coast (PADD I) and U.S. Gulf Coast (PADD III). For 100 percent production of RFG in PADD I during summer of the year 2000, the estimated reformulation costs increase moderately between VOC reductions of 20 and 30 percent. Reformulation costs are 9.0 cents per gallon at 20 percent VOC reduction and 15.2 cents per gallon at 30 percent VOC reduction. Reformulation costs increase rapidly to the right of an inflection in the cost curve (a cost knee) somewhere between VOC reductions of 30 and 32 percent. RVP reduction is the dominant VOC reduction mechanism. At high levels of VOC reduction, larger process capacity additions include fluid catalytic cracker (FCC) feed hydrofining, FCC gasoline fractionation, alkylation, ether production, and feed preparation for alkylation and etherification.

For the production of 50 percent RFG and 50 percent conventional gasoline in PADD III during summer of the year 2000, the estimated reformulation costs range from 3.5 cents per gallon (at 8 percent VOC reduction for RFG) to 15.4 cents per gallon (at 42 percent VOC reduction). Reformulation costs begin to increase rapidly after the RVP floor of 6.5 psi is reached, at a cost knee somewhere between an RFG VOC reduction of 35 and 40 percent. Even with anti-dumping

constraints, conventional gasoline appears to be an important sink which permits RFG to be blended with lower aromatics and sulfur contents. At high levels of VOC reduction, capacity additions include FCC gasoline fractionation, ether production, and feed preparation for alkylation and dimersol/polymerization units.

Estimated costs for 100 percent gasoline reformulation in PADD I are substantially greater than costs for 50 percent gasoline reformulation in PADD III. The cost difference suggests that the 100 percent RFG production assumption could be high for PADD I, and 50 percent RFG could be low for PADD III. The likely production shares in PADDs I and III could be estimated, given regional curves of cost versus production share and given the inter-regional delivery costs.

All RFGs of the PADD I and PADD III studies are NOX-compliant, given the DOE emissions models. However, half the study RFGs are not NOX-compliant, according to the October 1992 preliminary Complex Model of EPA. Refining studies with the EPA emissions equations could identify refining costs and problems unique to the EPA Complex Model. For example, with the EPA Complex Model, RVP reduction increases NOX emissions for gasolines with olefins contents greater than 9.2 percent.

In addition to the potentially large sensitivity of RFG production to different emissions models, RFG production is sensitive to the non-exhaust VOC share assumption for a particular VOC model. ORNL-RYM has also been used to estimate the sensitivity of RFG production to the cost of capital; to the RVP requirements for conventional gasoline; and to the percentage of RFG produced in a refining region.

Policy makers may use the reformulation cost knee to set emissions reduction targets, giving due consideration to the differences between model representations and actual refining operations. ORNL-RYM estimates that the reformulation cost knee for PADD I is about 15.2 cents per gallon with a VOC reduction of 30 percent; and the estimated cost knee for PADD III is about 5.5 cents per gallon with a VOC reduction of 35 percent. Reformulation cost estimates of various other studies range from 5 to 15 cents per gallon. In addition to these cost estimates, a 1991 poll of industry executives suggested that the CAAA could increase the cost of refining gasoline enough to boost prices by 6 to 10 cents per gallon.

1. THE CLEAN AIR ACT AMENDMENTS OF 1990

The Clean Air Act Amendments of 1990 (CAAA) will have far-reaching effects on the refining industry because, in addition to complying with all other CAAA provisions, refiners will have to modify, design, permit, and construct new units to produce mandated clean fuels. There are programs in the CAAA for oxygenated gasoline and for reformulated gasoline (RFG).

The oxygenated gasoline program requires that, beginning November 1, 1992, gasoline with a minimum oxygen content of 2.7 weight percent must be sold during winter months in about 40 cities not in compliance with carbon monoxide (CO) standards. RFGs are required by January 1, 1995, in nine areas with extreme or severe ozone pollution problems ("covered ozone nonattainment areas"). About 90 other cities with marginal, moderate, or serious ozone problems may "opt-in" to the RFG program.

The law specifies a formula and emissions performance standards for RFG, including:

A minimum oxygen content of 2 weight percent;

A maximum benzene content of 1 volume percent (the 1990 industry average gasoline contained 1.53 volume percent benzene);

No additives with heavy metals;

No increase in nitrogen oxide (NOX) emissions compared to present gasolines;

Beginning in 1995, a 15 percent reduction in volatile organic compounds (VOCs) during the high ozone season, and a 15 percent reduction in toxic air pollutants (TAPs) during the entire year, compared to 1990 levels. Beginning in the year 2000, VOC and TAP emissions are required to be at least 20 percent below 1990 levels. VOCs include all oxygenated and non-oxygenated hydrocarbons except for methane and ethane. TAPs consist of benzene, 1,3 butadiene, formaldehyde, acetaldehyde, and polycyclic organic matter.

The Environmental Protection Agency (EPA) used the negotiated rule making (Reg-Neg) process to allow parties who would be affected by the CAAA gasoline programs to negotiate an approach to the requirements of 1995 (Phase I). The CAAA requires a formal fuel certification procedure for demonstrating the emissions performance of a fuel. During the Reg-Neg workshop on fuel certification, the concept of emissions modeling was discussed. Emissions modeling provides a means for predicting the emissions performance of a gasoline, given other physical and chemical properties of the gasoline. On August 16, 1991, an agreement in principle established two emissions models: the Simple Model and the Complex Model.

The Simple Model is a set of equations that predicts emissions of VOCs and TAPs in terms of a gasoline's RVP, benzene, oxygen, and aromatics contents.

The Complex Model will be a set of equations that predicts emissions of VOCs, TAPs, and NOX in terms of the values of a larger number of gasoline properties. A preliminary Complex Model

published by EPA in October 1992 included RVP, T50, T90, benzene, oxygen, sulfur, aromatics, and olefins contents.

Gasoline producers may use either the Simple Model or the Complex Model or vehicle testing to certify the emissions performance of RFGs manufactured between January 1, 1995, and March 1, 1997. A Simple Model user must also cap the T90, sulfur, and olefins contents of RFG at the average values of his 1990 gasoline. After March 1, 1997, only the Complex Model or vehicle emissions testing will be used.

The nine areas in the extreme and serious ozone nonattainment categories currently comprise about 25 percent of the nation's gasoline market. However, because of the gasoline distribution system, surrounding areas will probably receive RFG as well. Taking these surrounding areas into consideration, the minimum market for RFG in 1995 is expected to be 21-23 percent of the current market.

Other areas are allowed to petition the EPA to opt-in to the RFG program. The most likely areas to request clean gasolines are the other less severe ozone non-attainment areas, which account for 20 to 35 percent of current gasoline demand. A significant motivation to enter the programs will come in November 1993, when State Implementation Plans (SIPs) are required. In the SIPs, states will have to demonstrate their strategies for achieving compliance with clean air standards. Using clean gasolines to reduce vehicular emissions could be more attractive than other alternatives. The total market for clean gasolines is uncertain, but it could exceed 50 percent by 1996-1997.¹

Besides requiring RFG in the covered ozone nonattainment areas, the CAAA requires that gasoline in all other areas not be any more polluting than it was in 1990. Without this "anti-dumping" provision, the potential exists for emissions from conventional gasoline (CG) to worsen as polluting fuel components are removed from and environmentally beneficial components are added to gasoline to be sold as RFG. For example, the national average benzene content of gasoline has been about 1.5 volume percent in recent summers. Since the benzene content of RFG cannot exceed 1.0 volume percent, it is conceivable that up to 0.5 percent volume percent benzene could be shifted to CG, increasing TAP emissions.²

In addition to constraints on the quality of gasoline, the CAAA also limits highway diesel fuel to a maximum sulfur content of 0.05 weight percent and a minimum cetane index of 40, effective October 1, 1993.³

With the passage of the CAAA, environmental regulations will constrain the market, define product composition and performance, influence technology, change consumer expectations of performance, and determine the feasibility of various production and supply options.¹ In short, domestic refinery operations will be driven by environmental regulations to a greater extent, and by the consumer to a lesser extent.⁴

During 1992, Oak Ridge National Laboratory (ORNL) performed petroleum refinery modeling and analysis necessary to support the Department of Energy (DOE) Office of Energy Demand Policy in an independent assessment of the likely costs and impacts on refineries of RFG requirements. The ORNL Refinery Yield Model (ORNL-RYM) was used, with input from the National Petroleum Council (NPC) refinery study. Concurrently with ORNL studies, the Advanced Computing Center

of Argenta (ACCA) performed estimation of Complex Model equations for the DOE Office of Energy Demand Policy.

The ORNL work included analysis of a number of issues which are discussed in this report, including:

Comparison of different emissions models;

Considerations in blending gasolines to satisfy emissions model constraints;

Regional production of gasolines blended to satisfy emission constraints, given a Complex Model;

Changes in gasoline production costs and blendstocks;

Process capacity investments required for the production of RFG; and

RFG production sensitivities.

2. THE ORNL REFINERY YIELD MODEL

2.1 ORNL-RYM Capabilities

Studies of RFG costs and refinery impacts were performed with ORNL-RYM, which is an enhanced personal computer version of the Refinery Yield Model of the Refinery Evaluation Modeling System.^{5,6,7,8} ORNL-RYM is a linear program that uses Haverly Systems software for matrix generation, optimization, and reporting.⁹

ORNL-RYM tracks octane, RVP, oxygen content, sulfur, benzene, aromatics, total olefins, distillation points, VOC, TAP, and NOX on all gasoline component streams. In separate data tables in ORNL-RYM, blending components for each gasoline grade are identified; blending values are assigned to each of up to 143 components; and blending targets (i.e., specifications with blending margins) are set.

The oxygen content of gasoline can be controlled by purchase of MTBE (methyl tertiary butyl ether), Oxinol, TBA (tertiary butyl alcohol), ethanol, or methanol; or by internal production (with alcohol purchase) of MTBE, TAME (tertiary amyl methyl ether), THME (tertiary hexyl methyl ether), ETBE (ethyl tertiary butyl ether), TAE (tertiary amyl ethyl ether), or THEE (tertiary hexyl ethyl ether).

Properties for distillates and jet fuels are handled conceptually the same as for gasoline. Properties can include gravity, aromatics content, paraffins content, naphthenes content, sulfur content, freezing point, luminometer number (which is correlated with smoke point), heat of combustion, hydrogen content, light cycle oil content, surface tension, pour point, cetane index, flash point, viscosities, RVP, distillation points, and diesel ignition improver content. The model also provides for several jet fuel additives for anti-icing, corrosion inhibition, and other functions.

Changes in crude feedstock are described in tables for crude quantity and assay. Changes in feedstock to individual process units are described in terms of different operation modes, each with different yields.

ORNL-RYM can be used to represent various regional refining configurations. Currently, ORNL-RYM includes 48 refining processes, which can be used to produce 40 different products from more than 100 crude oils. An investment module provides for the addition of processing capacity.

2.2 ORNL-RYM Simplifications

ORNL-RYM assumes that all refineries within a large region are interconnected. Consequently, ORNL-RYM has a tendency to over-optimize refinery operations. The over-optimization problem can sometimes be mitigated by focusing on changes in refining variables, rather than relying on the model to predict the exact value of variables. When ORNL-RYM is used to analyze uncharted refinery operations territory (e.g., production of RFG with very low VOC emissions), it is sometimes advisable to interpret results with a more qualitative perspective.

ORNL-RYM has several simplifications which are particularly important to consider in the analysis of RFG:

- (1) ORNL-RYM was updated in 1992 to represent the sulfur content property of gasolines.⁷ ORNL-RYM tends to produce RFGs with quite low sulfur contents, due largely to the production of low sulfur blendstocks by the FCC unit. The low sulfur property of RFGs may be coincident with refining strategies to meet emissions requirements by changing other properties, such as lowering the olefins content. Nevertheless, a review and possible revision are planned for sulfur content data for gasoline blendstocks.
- (2) Since ORNL-RYM is a regional model, it is assumed that all capacity investments are made in typical refining industry increments. Economies of scale are not applied to the ORNL-RYM investment purchases.⁷ Therefore, if a capacity addition is smaller than the typical refining industry increment, ORNL-RYM would understate the cost, contributing to over-optimization. An example of the consequences of this simplification is shown in Table 2.1.

Table 2.1. Example of investment scaling in ORNL-RYM

Assume that economies of scale for a new reformat fractionator are represented by:

$$\text{Cost}_{\text{actual}} = \text{Cost}_T * (\text{Size}/\text{Size}_T)^{0.7},$$

where

$\text{Cost}_{\text{actual}}$ = On-site cost of new reformat fractionator;

Cost_T = On-site cost of typical reformat fractionator;

Size = Capacity of new reformat fractionator;

Size_T = Capacity of typical reformat fractionator;

0.7 is the power factor correlating cost and capacity.

If $\text{Cost}_T = \$10,000,000$ for $\text{Size}_T = 20$ thousand barrels per day (MBD), then the estimated cost for a 15 MBD reformat fractionator is:

$$\text{Cost}_{\text{actual}} = \$10,000,000 * (15 \text{ MBD}/20 \text{ MBD})^{0.7},$$

$$\text{Cost}_{\text{actual}} = \$8,176,000.$$

However, the ORNL-RYM investment cost, which does not account for economies of scale, is simply:

$$\text{Cost}_{\text{ORNL-RYM}} = \text{Cost}_T * (\text{Size}/\text{Size}_T)$$

$$\text{Cost}_{\text{ORNL-RYM}} = \$10,000,000 * (15 \text{ MBD}/20 \text{ MBD}) = \$7,500,000.$$

In this example, ORNL-RYM has underestimated the actual investment cost by more than 8 percent.

- (3) Much of the control of aromatics in RFG will be via the naphtha reformer. Benzene reduction can be accomplished most simply by removing benzene precursors from reformer feed. In refining situations with ample ethers for octane improvement, the removed material can be blended directly into gasoline.¹⁰ ORNL-RYM does not have a representation of reformer feed fractionation to remove benzene precursors. Therefore, the ORNL-RYM refining options for benzene reduction in gasoline could be sub-optimal.
- (4) ORNL-RYM allows the modeler to blend to an optimal percentage distilled for a given temperature, but the model cannot blend to an optimal temperature for a specified percentage distilled. Finding the optimal T50 and T90 values for gasoline requires iteration. This inability of ORNL-RYM and other regional refinery linear programs could have important implications for blending gasoline to satisfy emission specifications as described in Section 3.

3. BLENDING GASOLINES TO SATISFY EMISSION SPECIFICATIONS

3.1 Emissions Models

ORNL-RYM and supporting software have been updated to blend gasolines to satisfy emissions constraints as defined by (1) the non-linear exhaust VOC model B1 of Advanced Computer Center of Argenta (ACCA);¹¹ (2) the non-linear NOX model D1 of ACCA;¹² and (3) the TAP and non-exhaust VOC models published in October 1992 by EPA.¹³ DOE sponsored the development of the ACCA models which are shown in Tables 3.1 and 3.2.

Table 3.1.
Exhaust VOC model B1 of Advanced Computer Center of Argenta¹¹

$$\begin{aligned} V(i) = & \exp [2.920763125 \\ & - 0.0112898176 \times \text{aromatics} \\ & - 0.0025357055 \times \text{olefins} \\ & + 0.028142957 \times \text{RVP} \\ & - 0.0159994212 \times \text{T50} \\ & - 0.022565112 \times \text{T90} \\ & + 0.0007281947 \times \text{sulfur} \\ & - 0.0123638914 \times \text{oxygen} \\ & - 0.0000630755 \times \text{aromatics} \times \text{T50} \\ & + 0.0000900669 \times \text{aromatics} \times \text{T90} \\ & + 0.00004849094 \times \text{T50} \times \text{T50} \\ & - 0.00000038557 \times \text{T50} \times \text{T90} \\ & + 0.00003495766 \times \text{T90} \times \text{T90} \\ & - 0.00000095498 \times \text{sulfur} \times \text{sulfur}] \end{aligned}$$

$$\text{VOC Exhaust (gm/mi)} = \text{baseline known mass} \times V(i)/V(\text{baseline})$$

$$\text{VOC Exhaust} = 0.41683 \times V(i)/0.24135$$

Table 3.2.
NOX model D1 of Advanced Computer Center of Argentina¹²

$$\begin{aligned}
 N(i) = \exp [& -2.43168044 \\
 & + 0.00844363 \times \text{aromatics} \\
 & + 0.00626083 \times \text{olefins} \\
 & + 0.01090873 \times \text{RVP} \\
 & + 0.00107160 \times \text{sulfur} \\
 & + 0.03058621 \times \text{oxygen} \\
 & - 0.00012928 \times \text{aromatics} \times \text{aromatics} \\
 & - 0.00081353 \times \text{aromatics} \times \text{oxygen} \\
 & - 0.00191451 \times \text{olefins} \times \text{oxygen} \\
 & + 0.00226251 \times \text{RVP} \times \text{oxygen} \\
 & - 0.00000148 \times \text{sulfur} \times \text{sulfur}]
 \end{aligned}$$

$$\text{NOX (gm/mi)} = \text{baseline known mass} \times N(i)/N(\text{baseline})$$

$$\text{NOX (gm/mi)} = 0.65999 \times N(i)/0.14253$$

The EPA non-exhaust VOC model of October 1992 is a function of RVP only as shown in Table 3.3. The EPA TAP model of October 1992 is listed in Appendix A.

Table 3.3.
EPA Non-exhaust VOC model of October 1992¹³

EPA proposes that non-exhaust emissions be modeled by the following relationships for Class B areas (typical of summer months and the warmer areas of the U.S., such as Arizona, California and Colorado):

$$\begin{aligned}\text{VOC DI} &= [0.003318 \times (\text{RVP}^2)] - [0.03475 \times \text{RVP}] + 0.09960 \\ \text{VOCHS} &= [0.007018 \times (\text{RVP}^2)] - [0.07351 \times \text{RVP}] + 0.2107 \\ \text{VOCRL} &= [0.006630 \times (\text{RVP}^2)] - [0.03047 \times \text{RVP}] + 0.02377 \\ \text{VOCRF} &= [0.0009804 \times (\text{RVP}^2)] - [0.008922 \times \text{RVP}] + 0.05877 \\ \text{VOCNE1} &= \text{VOC DI} + \text{VOCHS} + \text{VOCRL} + \text{VOCRF}\end{aligned}$$

where

RVP = Reid vapor pressure of the fuel, in pounds per square inch, and the range of applicability of RVP is 7 psi to 10 psi

VOC DI = Diurnal nonmethane, nonethane VOC emissions, in grams per mile

VOCHS = Hot soak nonmethane, nonethane VOC emissions, in grams per mile

VOCRL = Running loss nonmethane, nonethane VOC emissions, in grams per mile

VOCRF = Refueling nonmethane, nonethane emissions, in grams per mile

VOCNE1 = Non-exhaust emissions of volatile organic compounds in Class B areas, in grams per mile

Similarly, EPA proposes that non-exhaust emissions be modeled by the following relationships for Class C areas (typical of summer months and more moderate areas, such as Connecticut, Delaware, and Illinois):

$$\begin{aligned}\text{VOC DI} &= [0.003917 \times (\text{RVP}^2)] - [0.04828 \times \text{RVP}] + 0.1626 \\ \text{VOCHS} &= [0.008284 \times (\text{RVP}^2)] - [0.1021 \times \text{RVP}] + 0.3439 \\ \text{VOCRL} &= [0.003756 \times (\text{RVP}^2)] - [0.01780 \times \text{RVP}] + 0.06580 \\ \text{VOCRF} &= [0.0009804 \times (\text{RVP}^2)] - [0.008922 \times \text{RVP}] + 0.05877 \\ \text{VOCNE2} &= \text{VOC DI} + \text{VOCHS} + \text{VOCRL} + \text{VOCRF}\end{aligned}$$

where

VOCNE2 = Non-exhaust emissions of volatile organic compounds in Class C areas, in grams per mile

3.2 Representation of Non-linear Emissions Models in a Linear Program

Since ORNL-RYM is a linear program, a method to represent non-linear emissions models within ORNL-RYM had to be devised.

An ORNL study suggested that gasoline component emission blending values can be estimated in terms of the emission blending targets (specifications) for the product gasoline. The component blending values can be calculated before the refinery linear program solution process begins. A possible fortunate result is that the set of component blending values could be unique if there are unique regulation values for VOC, NOX, and TOX. The gasoline component emission blending values derived by this method appear to be valid if there is little or no give-away for the gasoline blending targets.¹⁴

Another method of representation of non-linear emissions models in a refinery linear program assumes that an emission value can be represented as a base emission value plus small linear emissions changes due to small changes in gasoline properties. The method, proposed by Bob Warden of Chevron, U.S.A., consists of a sequence of steps:

Step 1: Choose a base gasoline.

The base gasoline might have the following base PROPERTY values: oxygen=2.1; RVP=7.2; sulfur=140; aromatics=25; olefins=10; T50=200; T90=320; benzene=0.7; VOC=0.5664.

Step 2: Develop the blending equation (only the derivation for VOC for gasoline in the Class C area is illustrated).

$$\begin{aligned} \text{VOC} = & \text{VOC}_{\text{base}} \\ & + (\Delta\text{VOC}/\Delta\text{oxygen}) \times (\text{oxygen} - \text{oxygen}_{\text{base}}) \\ & + (\Delta\text{VOC}/\Delta\text{RVP}) \times (\text{RVP} - \text{RVP}_{\text{base}}) \\ & + (\Delta\text{VOC}/\Delta\text{sulfur}) \times (\text{sulfur} - \text{sulfur}_{\text{base}}) \\ & + (\Delta\text{VOC}/\Delta\text{aromatics}) \times (\text{aromatics} - \text{aromatics}_{\text{base}}) \\ & + (\Delta\text{VOC}/\Delta\text{olefins}) \times (\text{olefins} - \text{olefins}_{\text{base}}) \\ & + (\Delta\text{VOC}/\Delta\text{T50}) \times (\text{T50} - \text{T50}_{\text{base}}) \\ & + (\Delta\text{VOC}/\Delta\text{T90}) \times (\text{T90} - \text{T90}_{\text{base}}) \\ & + (\Delta\text{VOC}/\Delta\text{benzene}) \times (\text{benzene} - \text{benzene}_{\text{base}}) \end{aligned}$$

The $\Delta\text{VOC}/\Delta\text{PROPERTY}$ is an original coefficient (W_{original}).

For example, to determine $(\Delta\text{VOC}/\Delta\text{RVP})$ for the base gasoline in Step 1 (RVP=7.2 and VOC=0.5664), calculate VOC for that gasoline with RVP decreased by 0.1 psi (RVP=7.1 and VOC=0.5589):

$$(\Delta\text{VOC}/\Delta\text{RVP}) = (0.5664 - 0.5589)/(7.2 - 7.1) = 0.075$$

Step 3: Solve the linear program using the VOC constraint equation. For example,

$$\text{VOC} \leq 0.5524 \text{ (for a 30 percent VOC reduction)}$$

$$\begin{aligned} \text{VOC} = & 0.5664 \\ & - 0.004111 \times (\text{oxygen-2.1}) \\ & + 0.07500 \times (\text{RVP-7.2}) \\ & + 0.001543 \times (\text{sulfur-140}) \\ & + 0.001634 \times (\text{aromatics-25}) \\ & - 0.0008430 \times (\text{olefins-10}) \\ & + 0.0004816 \times (\text{T50-200}) \\ & + 0.0005981 \times (\text{T90-320}) \\ & + 0 \times (\text{benzene-0.7}) \end{aligned}$$

One way of representing the latter equation is to calculate the VOC values for each gasoline blendstock and load the values in a gasoline component blending table. ORNL-RYM does not provide for T50 and T90 blending values, so the modeler must assure that $(\text{T50}-\text{T50}_{\text{base}})$ and $(\text{T90}-\text{T90}_{\text{base}})$ equal zero.

Step 4: Given the linear program solution PROPERTY values, calculate the actual VOC using the emissions models. This step confirms whether the solution satisfies the VOC constraint.

Step 5: Given the linear program solution PROPERTY values, calculate new coefficients (W_{new}). Compare the original (W_{original}) and the new (W_{new}) coefficients for each PROPERTY.

Specify the unacceptable error percentage = ER%.

If $100\% \times |(W_{\text{original}} - W_{\text{new}})/W_{\text{original}}| > \text{ER}\%$, then go to Step 6. If not, then

ACCEPT LINEAR PROGRAM SOLUTION and STOP.

Step 6: Choose a new base gasoline with PROPERTY values equal to the linear program solution values. Go to Step 2.

Preliminary assessments showed that the Warden method performed acceptably and had implementation advantages.¹⁵ Computer programs were written to compute the $\Delta\text{VOC}/\Delta\text{PROPERTY}$, $\Delta\text{NOX}/\Delta\text{PROPERTY}$, and $\Delta\text{TAP}/\Delta\text{PROPERTY}$ coefficients, and to compute emission blending values for the 143 gasoline blending components in ORNL-RYM.

With the Warden method, two or three iterations are typically required for convergence for a problem in which non-exhaust VOC reduction is the controlling mechanism, and the marginal reduction of VOC is achieved by RVP reduction.

When RVP cannot be reduced further, and exhaust VOC reduction becomes the controlling mechanism, convergence can be difficult to achieve. There is usually a sharp increase in the cost of reformulation at this point.

4. REGIONAL PRODUCTION OF REFORMULATED GASOLINE

4.1 PADD I RFG Production Analysis

The updated ORNL-RYM and supporting software have been used to estimate the gasoline costs and property impacts for producing 100 percent RFG in Petroleum Administration for Defense District I (PADD I, the U.S. East Coast) during summer of the year 2000, based on conditions of the NPC constant demand scenario F2 (with gasoline demand adjusted to account for fuel economy differences).^{16,17}

4.1.1 PADD I Assumptions

The average world oil price is assumed to be \$27.80 per barrel (66.2 cents per gallon, 1990 U.S. currency), the DOE middle price outlook for the year 2000. The average world oil price is used as the reference to set ORNL-RYM prices for individual crude oils and products, such as those listed in the Table 4.1. The hydrocarbon product price differentials in Table 4.1 have remained nearly constant despite a tenfold range of crude oil prices during the last twenty-five years, including the 1986 price collapse. The ORNL-RYM price of MTBE is based on the NPC refining study differential with respect to the expected price of gasoline.

Table 4.1. Product price differentials ¹⁸	
Product	Relationship
MTBE	35.0 cents per gallon over unleaded regular motor gasoline
Unleaded premium gasoline	4.0 cents per gallon over unleaded regular motor gasoline
Unleaded regular motor gasoline	3.5 cents per gallon over No. 2 fuel oil
Jet A	3.0 cents per gallon over No. 2 fuel oil
No. 2 fuel oil	8% over crude oil
No. 6 fuel oil (0.7% sulfur)	77% of No. 2 fuel oil
Bunker fuel (3% sulfur)	68% of No. 2 fuel oil

In the scenario, RFG is produced for a range of VOC reductions (14 to 34 percent reduction), relative to the summer baseline gasoline (summer baseline VOC for region C = 0.7891 gm/mi). Relative to the summer baseline, a minimum TAP reduction of 25 percent is required for RFG (maximum TAP for region C = 30.05 mg/mi); and no degradation of NOX is allowed (maximum NOX = 0.66 gm/mi).

4.1.2 PADD I Gasoline Costs and Quality Impacts

The 1990 gasoline properties estimated by ORNL-RYM are compared to National Petroleum Refiners Association (NPRA) survey properties for 1989 in Table 4.2.

Table 4.2. PADD I historical gasoline properties		
	1990 (ORNL-RYM)	1989 (NPRA Survey) ¹⁹
RVP, psi	9.9	9.9
Aromatics, vol %	35.1	32.5
Benzene, vol %	1.4	NA
Olefins, vol %	16.3	17.8
Sulfur, ppm	339	448
T50, °F	221	206
T90, °F	333	337
Oxygen, wt %	0.42	0.42
Specific gravity	0.7454	0.7484
VOC, gm/mi	0.9738	0.9559
NOX, gm/mi	0.6967	0.6964
TAP, mg/mi	53.12	NA

Figs. 4.1 through 4.11 summarize the gasoline cost and property impacts for year 2000 RFG VOC reductions ranging from 14 percent to 34 percent.

Fig. 4.1 shows that reformulation costs increase moderately between VOC reductions of 20 and 30 percent. *Reformulation costs are 9.0 cents per gallon at 20 percent VOC reduction and 15.2 cents per gallon at 30 percent VOC reduction.* Costs account for fuel economy losses in RFG, and costs are relative to a baseline case with production of 100 percent CG with 8.7 psi RVP.

In Fig. 4.1, the cost for benzene control, oxygenate addition, and 25 percent TAP reduction, with no constraint on VOC, is 8.1 cents per gallon; the associated unconstrained VOC reduction is 14 percent.

Fig. 4.1 also shows that *reformulation costs increase rapidly after a cost "knee" somewhere between an RFG VOC reduction of 30 and 32 percent.*

Fig. 4.2 suggests that all RFGs are NOX-compliant in PADD I, given the NOX emissions model D1 of ACCA. However, study results would have been different for NOX and exhaust VOC models published by EPA in October 1992. The EPA NOX model is listed in Appendix A.

Table 4.3 shows that *several RFGs are not NOX-compliant, according to the October 1992 preliminary Complex Model of EPA*. Table 4.3 also shows that EPA-derived VOC reductions are generally smaller. A similar study with EPA emissions equations could identify refining costs and problems unique to the EPA Complex Model.

Table 4.3. Emissions comparisons for PADD I RFGs						
	Study gasoline observation number					
	#1	#2	#3	#4	#5	#6
Exhaust VOC emissions, gm/mi (ACCA model B1)	.3399	.3246	.3287	.3218	.3298	.3258
Exhaust VOC emissions, gm/mi (EPA model)	.3694	.3801	.3768	.3733	.3351	.3309
Total VOC % reduction (ACCA model B1 + EPA non-exhaust VOC model)	14	20	25	30	32	34
Total VOC % reduction (EPA models)	10	13	19	24	32	33
NOX emissions, gm/mi (ACCA model D1)	.6119	.5908	.58501	.5818	.5719	.5688
NOX emissions, gm/mi (EPA model). Shaded cells are non-compliant.	.6345	.6442	.6757	.7040	.6706	.7095
NOX % reduction (ACCA model D1)	7	10	11	12	13	14
NOX % reduction (EPA model)	4	2	-2	-7	-2	-8

The TAP-VOC relationship is shown in Fig. 4.3. TAP is a binding emissions constraint in all cases.* VOC is a binding emissions constraint in all cases except 14 percent VOC reduction.

The RVP-VOC relationship is plotted in Fig. 4.4. *RVP reduction is the dominant VOC reduction mechanism*. Table 4.3 shows that exhaust VOC (ACCA model B1) is nearly constant for VOC reductions greater than 20 percent, indicating that the RVP-dependent non-exhaust VOC is being reduced. However, RVP drops only to 6.6-6.7 psi, because of modeled constraints on naphtha markets. These constraints may contribute to sub-optimization in the analysis. For RVP to reach the allowable floor of 6.5 psi, naphtha would have to be dumped.

*RFG TAP values are slightly scattered in Fig. 4.3 due to the convergence method discussed in Section 3.2. As suggested by Step 4 of the method, there can be slight differences between the model-derived emissions value and the actual emissions values. For this reason, it is possible for all RFG TAP values to be binding at a single value in the model, while the actual TAP values are slightly different. All RFG TAP values satisfy the actual 25 percent reduction requirement.

Figs. 4.5, 4.7, 4.8, and 4.9 show sharp downward trends for aromatics, olefins, benzene, and T90 to the right of the cost knee.

As discussed in Section 2.2, ORNL-RYM tends to understate the sulfur content property of RFG. In Fig. 4.6, sulfur falls from about 100 ppm at 14 percent VOC reduction to about 60 ppm for VOC reductions of 20 percent or greater. The apparent reason for the drop from 100 ppm to 60 ppm will be explained using the change from 14 to 20 percent VOC reduction:

RVP is reduced by rejecting pentanes (e.g., isopentane falls from 4.1 to 2.0 percent) and by introducing relatively-lower-RVP components such as C5 alkylate and dimate. TAME replaces a small percentage of MTBE.

FCC operations are changed to provide greater output of amylenes (for C5 alkylate and TAME), and FCC output of propylene is also increased (propylene is used for dimate production).

A greater percentage of FCC feed is hydrofined, to increase the yield of C5 olefins. Hydrofining contributes to the production of RFG-blend-naphthas with average sulfur content reduced by half.

The model has selected a non-exhaust VOC reduction strategy (RVP reduction) which also has small exhaust VOC reduction benefits (through sulfur reduction, with possible over-optimization in the model).

Figs. 4.10 and 4.11 show that T50 and specific gravity have upward trends, except for a drop in specific gravity at 34 percent VOC reduction.

4.1.3 PADD I Gasoline Blendstocks

Table 4.4 shows recent gasoline blendstocks in PADD I. Table 4.5 summarizes PADD I gasoline blendstocks for the study cases.

Table 4.4. PADD I average gasoline blendstocks for 4/1/89 - 9/30/89 ¹⁹	
Blendstock	Percent
Butane	3.8
Reformate	24.3
Straight run naphtha	4.1
C5+ isomerate	
FCC naphtha	42.3
Coker naphtha	
Hydrocrackate	
Alkylate	9.4
Polymer gasolines	0.9
Dimate	
MTBE	1.6
Toluene/xylene	
Natural gasoline	
Pyrolysis gasoline	
Raffinates	1.4
Other	12.2

Table 4.5 shows that to the right of the cost knee, RFG is blended with decreased percentages of FCC naphtha and increased percentages of alkylate. The percentage of reformate blended to RFG peaks in the vicinity of the cost knee and then drops sharply. For VOC reductions greater than 20 percent, there are decreasing percentages of straight run naphtha and isopentane (C5 rejection for RVP control). Disposal of light naphthas is limited by modeled constraints on markets (e.g., naphthas for petrochemicals) and is a reason for RVP dropping only to 6.6-6.7 psi. For RVP to reach the allowable floor of 6.5 psi, naphtha would have to be dumped. The percentage of MTBE gradually falls, with oxygen provided by heavier ethers included in the "Other" row.

Table 4.5. RFG blendstocks in PADD I for the year 2000 (percent)						
Blendstock	RFG VOC Reduction (percent)					
	14	20	25	30	32	34
Butane	2.0	2.0	2.0	2.0	2.0	2.0
Reformate	18.4	19.3	20.5	24.8	25.6	13.4
Straight run naphtha		3.8	2.7	0.9		
Isopentane	4.1	2.0				
C6 isomerate	4.9	3.3	3.8	5.3	3.3	7.2
FCC naphtha	45.4	42.6	42.1	33.8	25.7	29.1
Coker naphtha						
Hydrocrackate				0.8	3.2	2.2
Alkylate	12.9	12.2	14.4	14.5	23.1	27.6
Polymer gasolines	0.5					
Dimate		2.7	2.1	3.9		
MTBE	11.6	10.7	8.5	6.5	6.6	3.1
Toluene/xylene						
Natural gasoline						
Pyrolysis gasoline						
Raffinates					0.5	0.6
Other	0.1	1.3	3.9	7.6	10.1	14.7

4.1.4 PADD I Process Capacity Additions

Table 4.6 summarizes process capacity additions with increasing VOC reduction for RFG. At high levels of VOC reduction, larger capacity additions include FCC feed hydrofining, gasoline fractionation, alkylation, ether production, and feed preparation for alkylation and etherification.

As previously noted, to the right of the cost knee, RFG is blended with decreased percentages of FCC naphtha. However, FCC utilization is constant (at the maximum 91 percent) over the range of VOC reductions. With increasing VOC reduction, FCC and related operations are driven in part by the production of C5 olefins for alkylation and for the production of TAME. FCC hydrofining increases the yield of C5+ FCC product, which is fractionated to produce C5 olefins. Alkylation is also supported by the production of amylene by C5 dehydrogenation and by the production of isobutane by naphtha cracking.

Table 4.6.
Process capacity additions in PADD I
for the year 2000 (MBD)

(Base capacity is 1992 in-place plus announced additions)

Process	RFG VOC Reduction (percent)					
	14	20	25	30	32	34
Butene isomerization for alkylation	28	35	36	36	34	43
Alkylation	12	6	22	19	78	107
Ether plant	12	23	41	57	45	64
Hydrogen plant	4	4	3	1	9	15
Distillate deep hydrotreating	9	9	10	9	22	19
FCC feed hydrofiner	241	246	237	180	160	284
FCC gasoline fractionation	8	36	41	158	318	335
Naphtha cracker	59	60	60	51	104	155
Hydrocracker				12	52	47
C2/C5 dehydrogenation		4	18	26	16	35
Dimersol		18	14	26		
C4 isomerization			10	9	24	33
C5/C6 isomerization	20		6	25		50
Visbreaker	6	9	9	9	52	66

4.2 PADD III RFG Production Analysis

4.2.1 PADD III Assumptions

ORNL-RYM has been used to estimate the gasoline costs and property impacts for producing 50 percent RFG and 50 percent CG in PADD III during summer of the year 2000, based on conditions of the NPC constant demand scenario F2 (with gasoline demand adjusted to account for fuel economy differences).^{16,17} The raw material and product value assumption basis is the same as discussed in Section 4.1.1 for PADD I.

In the scenario, RFG is produced for a range of VOC reductions (8 to 42 percent reduction), relative to the summer baseline gasoline (summer baseline VOC for 60 percent Region B and 40 percent Region C = 0.8457 gm/mi).^{*} Relative to the summer baseline, a minimum TAP reduction

^{*}Baseline gasoline RVP is assumed to be 8.7 psi for both Class B and Class C areas. In other literature, the baseline RVP for Class B areas may be 7.8 psi.²⁰ Different baseline RVP assumptions will yield different percentage emissions reductions for the same test gasoline.

of 25 percent is required for RFG (maximum TAP = 30.53 mg/mi); and no degradation of NOX is allowed (maximum NOX = 0.66 gm/mi).

CG is produced, subject to no degradation of VOC, TAP, and NOX, relative to ORNL-RYM-derived properties of 1990 gasoline in PADD III. The 1990 model-derived gasoline properties are compared to NPRA survey properties for 1989 in Table 4.7.

Table 4.7. PADD III historical gasoline properties		
	1990 (ORNL-RYM)	1989 (NPRA Survey) ¹⁹
RVP, psi	9.4	9.4
Aromatics, vol %	32.1	31.5
Benzene, vol %	1.4	NA
Olefins, vol %	11.3	12.2
Sulfur, ppm	228	260*
T50, °F	202	212
T90, °F	326	341
Oxygen, wt %	0.22	0.22
Specific gravity	0.7389	0.7467*
VOC, gm/mi	0.9334	0.9641
NOX, gm/mi	0.6572	0.6682
TAP, mg/mi	38.59	NA

*Because of missing entries in the NPRA table, value cannot be verified.

4.2.2 PADD III Gasoline Costs and Quality Impacts

Figs. 4.12 through 4.23 show gasoline cost and property impacts for RFG VOC reductions ranging from 8 percent to 42 percent.

Fig. 4.12 shows that *reformulation costs range from 3.5 cents per gallon (at 8 percent VOC reduction for RFG) to 15.4 cents per gallon (at 42 percent VOC reduction for RFG)*. These costs account for fuel economy losses in RFG and for fuel economy changes in CG (e.g., the fuel economy of CG changes with gravity; see Fig. 4.23). Costs are relative to a baseline case with 100 percent CG with 8.7 psi RVP.

In Fig. 4.12, the *cost for benzene control, oxygenate addition, and 25 percent TAP reduction, with no constraint on VOC, is 3.5 cents per gallon*; the associated unconstrained VOC reduction is 8 percent.

Together, Figs. 4.12 and 4.16 show that *reformulation costs begin to increase rapidly after the RVP floor of 6.5 psi is reached, at a cost knee somewhere between an RFG VOC reduction of 35 and 40 percent*.

In Figs. 4.13, 4.14, and 4.15, VOC, NOX, and TAP are plotted in relation to the VOC reduction in RFG. For RFG, VOC is the binding emissions constraint in all cases. For CG, TAP is a binding constraint in all except the case for 8 percent reduction of RFG VOC.* For CG, NOX is a binding constraint only in the case for 35 percent reduction of RFG VOC.

Over the VOC reductions plotted in Fig. 4.17, the pooled aromatics content drops from 30 percent to 26 percent. *Even with anti-dumping constraints, the CG appears to be an important sink which permits RFG to be blended with lower aromatics content.*

Over the VOC reductions plotted in Fig. 4.18, the pooled sulfur content drops from 217 ppm to 187 ppm. *Even with anti-dumping constraints, the CG appears to be an important sink which permits RFG to be blended with lower sulfur content* (as discussed in Section 2.2, ORNL-RYM tends to understate the sulfur content property of RFG).

In Fig. 4.19, the pooled olefins content is fairly constant (in the 8.5 to 8.9 percent range) up to 39 percent RFG VOC reduction, with a sharp increase to 12.9 percent in the case for 42 percent reduction of RFG VOC.

*CG TAP values are slightly scattered in Fig. 4.15 due to the convergence method discussed in Section 3.2. As suggested by Step 4 of the method, there can be slight differences between the model-derived emissions value and the actual emissions values. For this reason, it is possible for all CG TAP values to be binding at a single value in the model, while the actual TAP values are slightly different. All CG TAP values satisfy the actual requirement for no degradation in TAP relative to the 1990 PADD III gasoline.

Figs. 4.17 and 4.19 show that, at 42 percent VOC reduction, RFG has very low aromatics (12.6 percent) and very high olefins (21.2 percent), with both property values beyond the range of applicability of the EPA Complex Model of October 1992.*

Over the range of VOC reductions plotted in Fig. 4.20, the pooled benzene content drops from 1.28 percent to 1.11 percent.

Figs. 4.16, 4.21, and 4.22 suggest that, with increasing VOC reduction, RFG production is pinched from both ends of the distillation curve, given the reduction in RVP, increase in T50, and decrease in T90.

4.2.3 PADD III Gasoline Blendstocks

Table 4.8 shows recent gasoline blendstocks in PADD III. Tables 4.9 through 4.11 summarize PADD III gasoline blendstocks for the study cases.

Table 4.8. PADD III average gasoline blendstocks for 4/1/89 - 9/30/89 ¹⁹	
Blendstock	Percent
Butane	3.0
Reformate	23.4
Straight run naphtha	2.7
C5+ isomerate	3.4
FCC naphtha	40.6
Coker naphtha	0.4
Hydrocrackate	0.8
Alkylate	13.2
Polymer gasolines	0.1
Dimate	0.2
MTBE	1.2
Toluene/xylene	1.3
Natural gasoline	0.7
Pyrolysis gasoline	0.7
Raffinates	1.8
Other	6.6

*For the EPA Complex Model of October 1992, the applicable aromatics range is 20 to 45 percent, and the olefins range is 2 to 20 percent.

For the combined gasoline pool blendstocks, Table 4.9 shows that, with increasing VOC reduction for RFG, reformat peaks at 35 percent RFG VOC reduction, and then falls sharply to the right of the cost knee. There are decreasing percentages of straight run naphtha and FCC naphtha. To the right of the cost knee, there are increasing percentages of hydrocrackate, polymer gasolines and dimate (the latter two blendstocks with almost zero aromatics/benzene and with high olefins content). To the right of the cost knee, the percentage of MTBE falls (compensated by heavier ethers included in the "Other" row).

Table 4.9.
Combined gasoline pool blendstocks in PADD III
for the year 2000 (percent)

Blendstock	RFG VOC Reduction (percent)						
	8	20	25	31	35	39	42
Butane	2.4	2.0	2.0	2.0	2.0	2.0	2.0
Reformat	29.7	31.3	32.3	32.8	35.1	31.7	21.6
Straight run naphtha	7.3	7.3	7.5	5.0	4.2	3.3	3.2
C5+ isomerate	5.5	5.5	5.5	5.5	5.5	5.5	6.0
FCC naphtha	30.6	30.3	30.0	29.9	28.8	24.0	23.9
Coker naphtha							
Hydrocrackate	3.5	3.0	2.6	4.9	3.9	6.4	6.7
Alkylate	14.0	13.6	13.1	13.0	12.8	13.7	14.3
Polymer gasolines	1.0	1.0	1.0	1.0	1.0	0.6	2.2
Dimate	0.1	0.1	0.1	0.1	0.1	2.6	5.6
MTBE	5.8	5.8	5.8	5.8	5.8	4.4	2.2
Toluene/xylene							
Natural gasoline							
Pyrolysis gasoline							
Raffinates					0.2	1.2	2.6
Other					0.4	4.6	9.9

Table 4.10 shows that, compared with the combined gasoline pool, conventional gasoline is generally high in reformate and FCC naphtha, and low in alkylate. With increasing VOC reduction for RFG, there are decreasing percentages of reformate and straight run naphtha. FCC naphtha peaks at 35 percent RFG VOC reduction, and then falls to the right of the cost knee. To the right of the cost knee, there are sharply increased percentages of C5+ isomerate and hydrocrackate, and decreasing percentages of alkylates.

Only 2 percent normal butane is blended to the CGs in Table 4.10 because of limited availability of C4s (normal butane and isobutane).^{*} Relative to 1990, the volume of C4s produced by the ORNL-RYM refinery in the year 2000 falls by an amount greater than the volume of C4s released in the production of low-RVP RFG. In the ORNL-RYM analysis for 1990, the hydrocracker is operated to produce naphthas, for reformer feed and for blending into gasoline. However, in the year 2000, the hydrocracker is switched to distillate modes to produce large volumes of (low sulfur) hydrocrackate for blending into low sulfur diesel fuel (the sulfur maximum for year 2000 diesel fuel is 0.05 weight percent versus the 1990 blending target of 0.25 weight percent). In the distillate modes, C4s produced by the hydrocracker fall to about 9 volume percent of feed, versus 20 percent of feed in the year 1990. Compared to 1990, C4s produced by the hydrocracker fall by about 50 MBD in year 2000. Compared to 1990, if all gasolines are blended with 2 percent butane in the year 2000, about 30 MBD of butane is released. Other reasons for reduced C4 availability include reduced crude throughput.

^{*}The maximum volume of purchased C4s is limited to the volume purchased in the constant demand scenario.

Table 4.10.
Conventional gasoline blendstocks in PADD III
for the year 2000 (percent)

Blendstock	RFG VOC Reduction (percent)						
	8	20	25	31	35	39	42
Butane	2.0	2.0	2.0	2.0	2.0	2.0	2.0
Reformate	42.9	42.8	40.8	37.9	31.5	32.1	28.1
Straight run naphtha	9.7	9.2	9.1	8.3	6.6	6.6	6.4
C5+ isomerate	4.2	5.1	5.1	5.1	5.1	11.1	11.8
FCC naphtha	23.8	29.5	31.2	34.6	41.0	37.5	38.8
Coker naphtha							
Hydrocrackate	7.1	6.1	5.2	4.7	2.7	6.4	6.4
Alkylate	10.2	5.4	6.6	7.5	10.5	1.6	0.3
Polymer gasolines							
Dimate	0.2						
MTBE							
Toluene/xylene							
Natural gasoline							
Pyrolysis gasoline							
Raffinates							
Other					0.6	2.8	6.2

Table 4.11 shows that, compared with the combined gasoline pool, RFG is generally low in reformat and FCC naphtha, and high in alkylate and ethers. With increasing VOC reduction for RFG, reformat peaks at 35 percent VOC reduction, and then falls sharply to the right of the cost knee; and there are decreasing percentages of straight run naphtha (C5 rejection for RVP control) and FCC naphtha. To the right of the cost knee, C5+ isomerate percentages fall sharply; there are increasing percentages of hydrocrackate, polymer gasolines and dimate (the latter two blendstocks with almost zero aromatics/benzene and with high olefins content); and the percentage of MTBE falls, compensated by heavier ethers included in the "Other" row.

<p>Table 4.11. RFG blendstocks in PADD III for the year 2000 (percent)</p>							
Blendstock	RFG VOC Reduction (percent)						
	8	20	25	31	35	39	42
Butane	2.9	2.0	2.0	2.0	2.0	2.0	2.0
Reformat	16.8	20.1	24.0	27.8	38.7	31.4	15.2
Straight run naphtha	5.0	5.4	6.0	1.8	1.8		
C5+ isomerate	6.8	6.0	6.0	6.0	6.0	0.1	0.3
FCC naphtha	37.3	31.2	28.8	25.3	16.9	10.8	9.3
Coker naphtha							
Hydrocrackate					5.2	6.5	7.0
Alkylate	17.7	21.6	19.6	23.4	15.1	25.5	28.1
Polymer gasolines	2.0	2.0	2.0	2.0	2.0	1.2	4.3
Dimate		0.2	0.2	0.2	0.2	5.2	11.0
MTBE	11.5	11.5	11.5	11.5	11.5	8.6	4.3
Toluene/xylene							
Natural gasoline							
Pyrolysis gasoline							
Raffinates					0.5	2.3	5.1
Other					0.2	6.3	013.5

4.2.4 PADD III Process Capacity Additions

Table 4.12 summarizes process capacity additions with increasing VOC reduction for RFG. At high levels of VOC reduction, capacity additions include FCC gasoline fractionation, ether production, and feed preparation for alkylation and dimersol/polymerization units.

<p>Table 4.12. Process capacity additions in PADD III for the year 2000 (MBD)</p> <p>(Base capacity is 1992 in-place plus announced additions)</p>							
Process	RFG VOC Reduction (percent)						
	8	20	25	31	35	39	42
Butene isomerization for alkylation	96	94	90	90	128	160	127
Ether plant	38	37	35	35	37	109	140
Distillate deep hydrotreating		4	5			3	
FCC feed hydrofiner							204
FCC gasoline fractionation					61	641	1208
Light gas cracker							26
C2/C5 dehydrogenation							30
Dimersol						83	179
Polymerization							38
C5/C6 isomerization							52
Fluid coker							83

4.3 PADD I and III RFG Production Summaries

4.3.1 PADD I RFG Production Summary

ORNL-RYM has been used to estimate the gasoline costs and property impacts for producing 100 percent RFG in PADD I during summer of the year 2000.

PADD I reformulation costs increase moderately between VOC reductions of 20 and 30 percent. Reformulation costs are 9.0 cents per gallon at 20 percent VOC reduction and 15.2 cents per gallon at 30 percent VOC reduction.

The PADD I cost for benzene control, oxygenate addition, and 25 percent TAP reduction, with no constraint on VOC, is 8.1 cents per gallon; the associated unconstrained VOC reduction is 14 percent.

Reformulation costs increase rapidly to the right of a cost knee somewhere between VOC reductions of 30 and 32 percent.

RVP reduction is the dominant VOC reduction mechanism.

To the right of the cost knee, RFG is blended with decreasing percentages of FCC naphtha and increasing percentages of alkylate. The percentage of reformate blended to RFG peaks in the vicinity of the cost knee and then drops sharply.

At high levels of VOC reduction, larger process capacity additions include FCC feed hydrofining, FCC gasoline fractionation, alkylation, ether production, and feed preparation for alkylation and etherification.

4.3.2 PADD III RFG Production Summary

ORNL-RYM has been used to estimate the gasoline costs and property impacts for producing 50 percent RFG and 50 percent CG in PADD III during summer of the year 2000.

PADD III reformulation costs range from 3.5 cents per gallon (at 8 percent VOC reduction for RFG) to 15.4 cents per gallon (at 42 percent VOC reduction).

The PADD III cost for benzene control, oxygenate addition, and 25 percent TAP reduction, with no constraint on VOC, is 3.5 cents per gallon; the associated unconstrained VOC reduction is 8 percent.

Reformulation costs begin to increase rapidly after the RVP floor of 6.5 psi is reached, at a cost knee somewhere between an RFG VOC reduction of 35 and 40 percent.

Even with anti-dumping constraints, CG appears to be an important sink which permits RFG to be blended with lower aromatics and sulfur contents.

RFG is generally low in reformate and FCC naphtha, and high in alkylate and ethers. CG is relatively high in reformate and FCC naphtha, and low in alkylate and ethers.

To the right of the cost knee, RFG is blended with sharply decreased percentages of reformate and C5+ isomerate; and with increased percentages of hydrocrackate, polymer gasoline and dimate.

At high levels of VOC reduction, capacity additions include FCC gasoline fractionation, ether production, and feed preparation for alkylation and dimersol/polymerization units.

4.3.3 Comparison of PADD Costs/Sensitivity to RFG Production Share

Estimated costs for 100 percent gasoline reformulation in PADD I are substantially greater than costs for 50 percent gasoline reformulation in PADD III. The cost difference suggests that the 100 percent RFG production assumption could be high for PADD I, and 50 percent RFG could be low for PADD III. The sensitivity of cost to RFG production share in PADD I is demonstrated by the ORNL-RYM estimates in Table 4.13. The likely production shares in PADDs I and III could be

estimated, given regional curves of cost versus production share and given the inter-regional delivery costs.

Table 4.13 shows that, in PADD I, 50 percent of the gasoline can be reformulated (with 30 percent VOC reduction) at a cost of 8.3 cents per gallon. As shown in Fig. 4.12, 50 percent of the gasoline in PADD III can be reformulated at the considerably lower cost of 4.6 cents per gallon.

Table 4.13. Reformulation cost versus RFG production share in PADD I (30 percent VOC reduction and 25 percent TAP reduction in RFG)	
RFG production share (percent)	Reformulation cost (cents per gallon of RFG)
100	15.2
75	10.6
50	8.3

Fig. 4.1.
PADD I reformulation cost versus VOC reduction

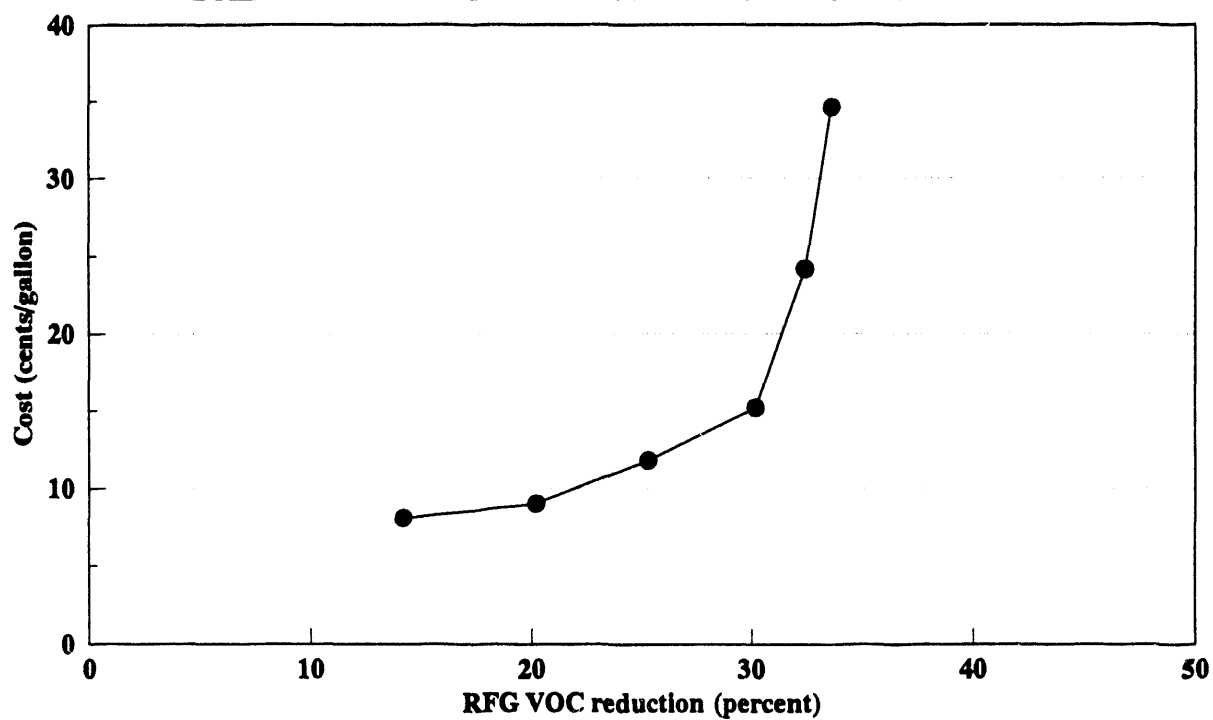


Fig. 4.2.
PADD I RFG NOX versus VOC reduction

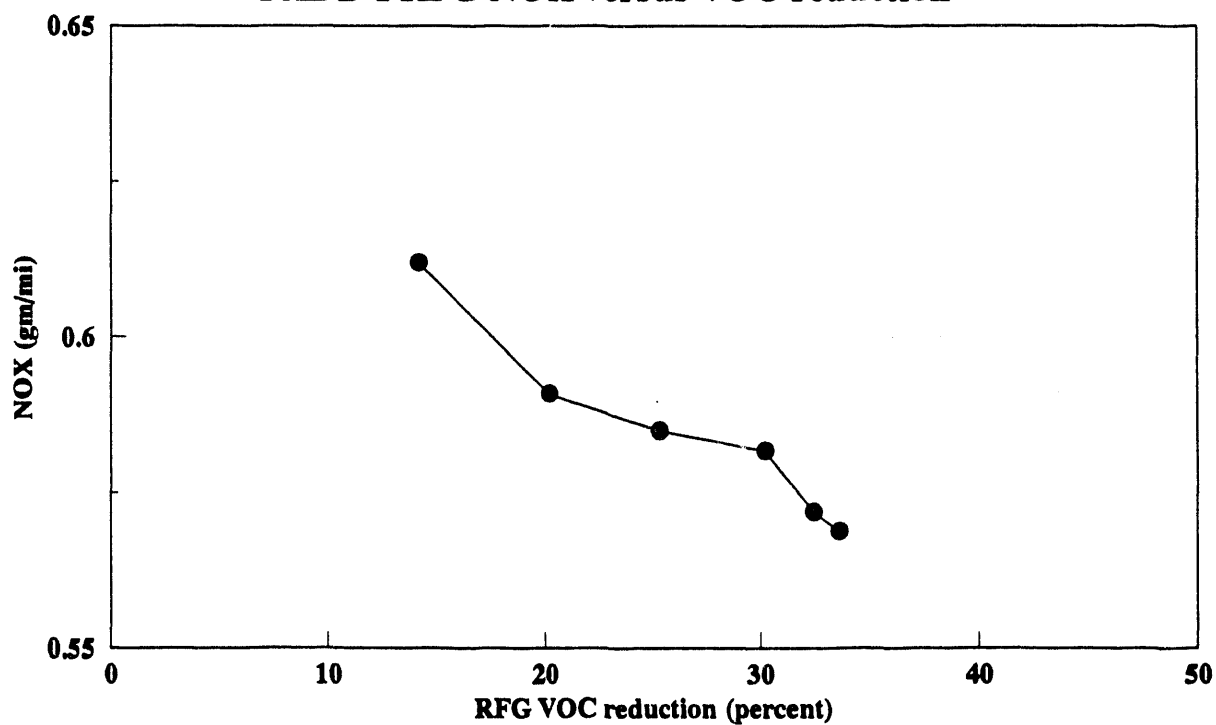


Fig. 4.3.
PADD I RFG TAP versus VOC reduction

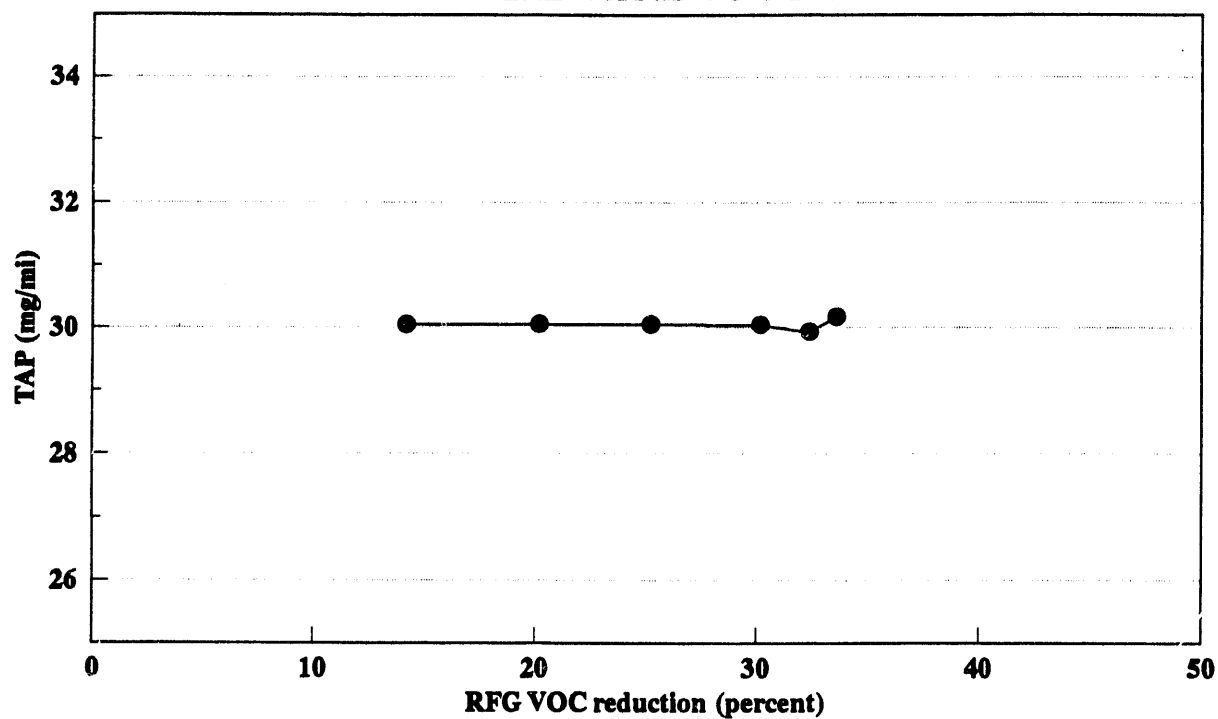


Fig. 4.4.
PADD I RFG RVP versus VOC reduction

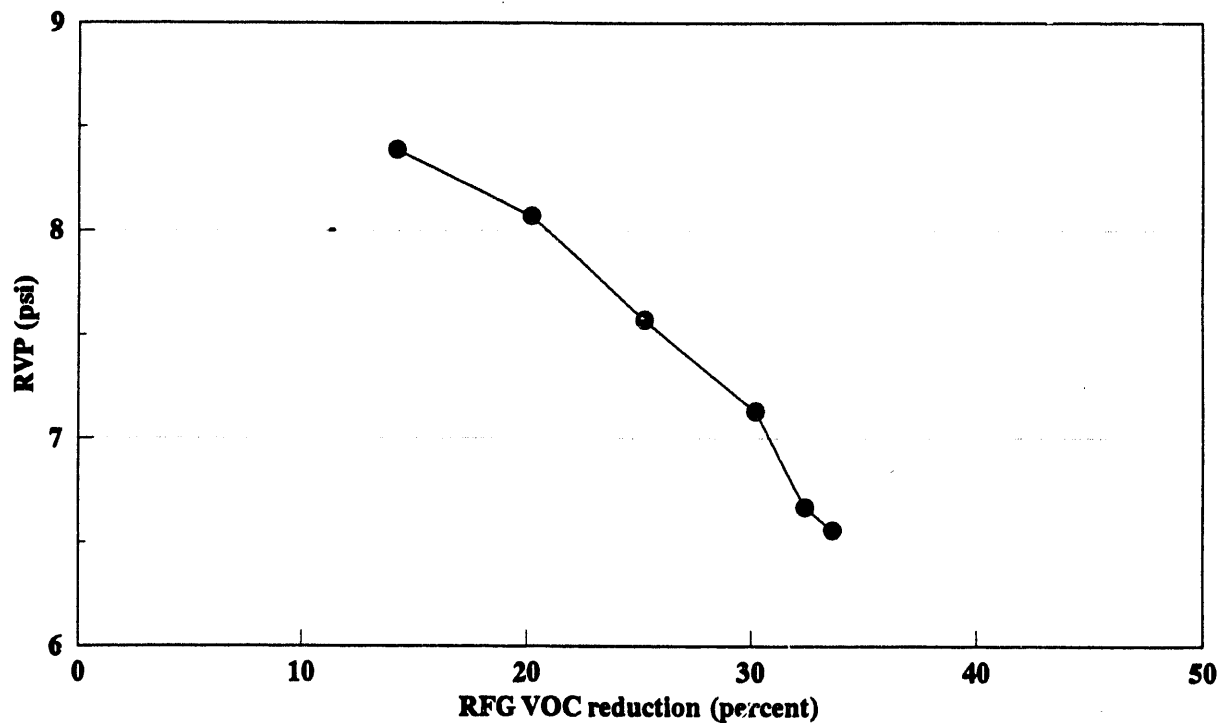


Fig. 4.5.
PADD I RFG aromatics versus VOC reduction

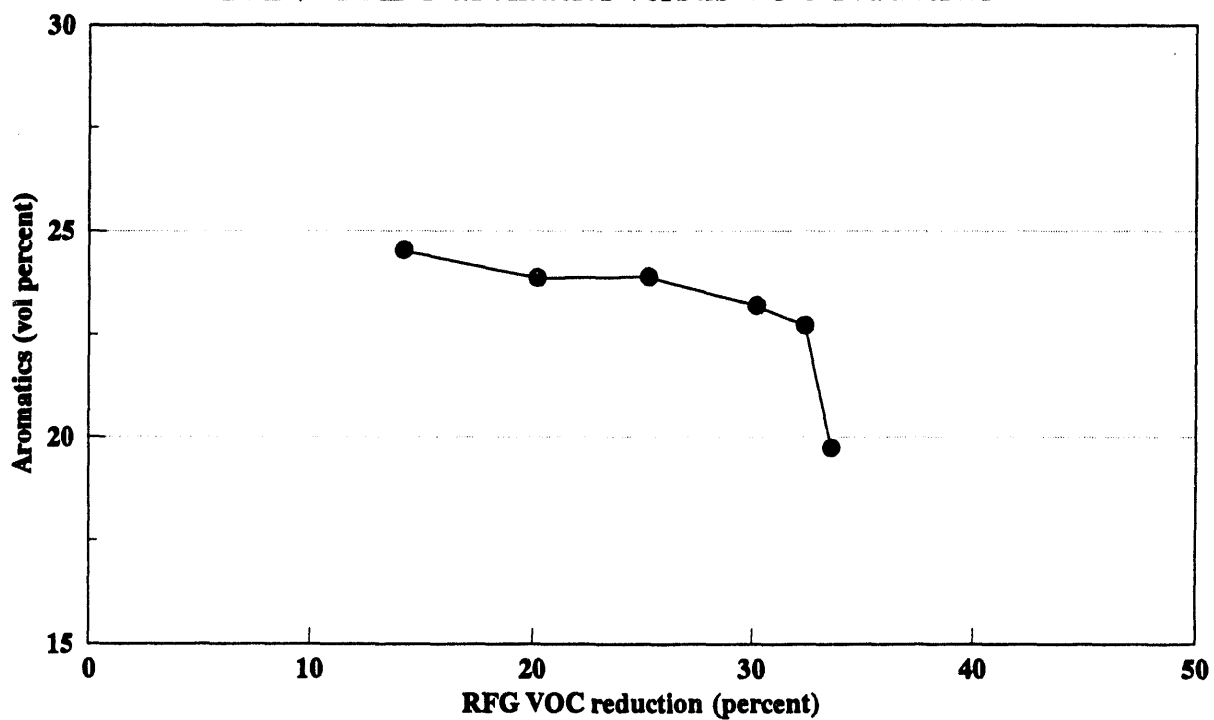


Fig. 4.6.
PADD I RFG sulfur versus VOC reduction

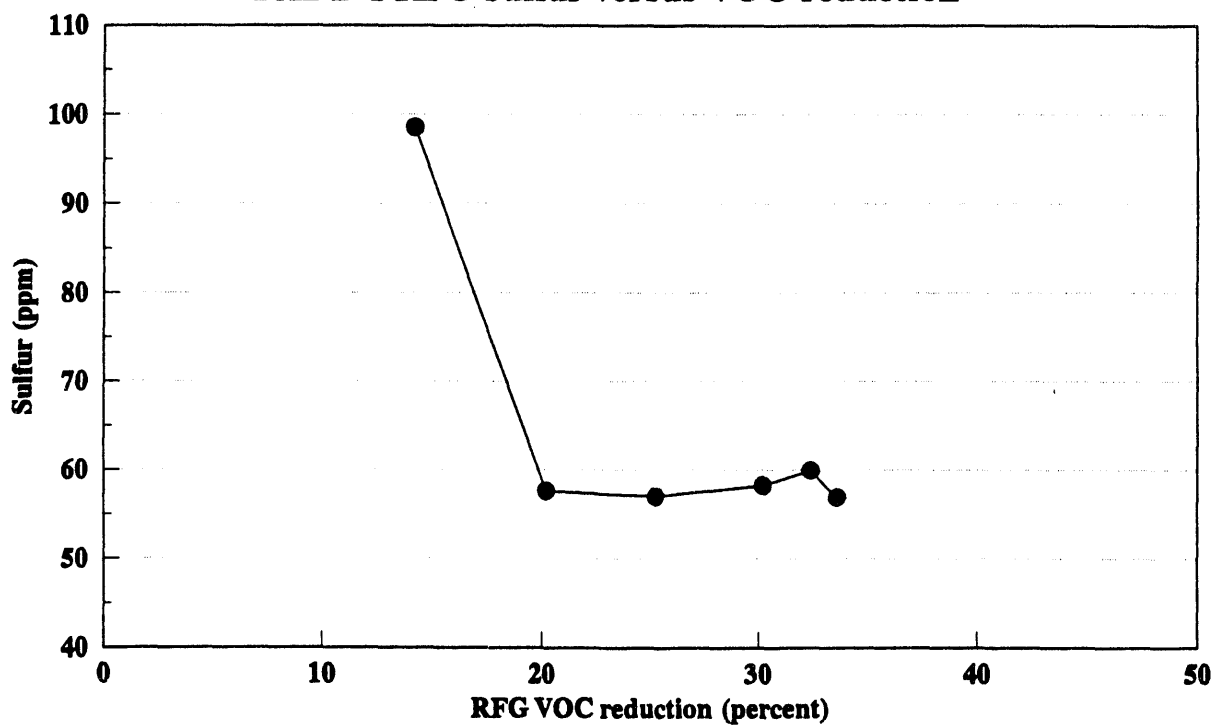


Fig 4.7.
PADD I RFG olefins versus VOC reduction

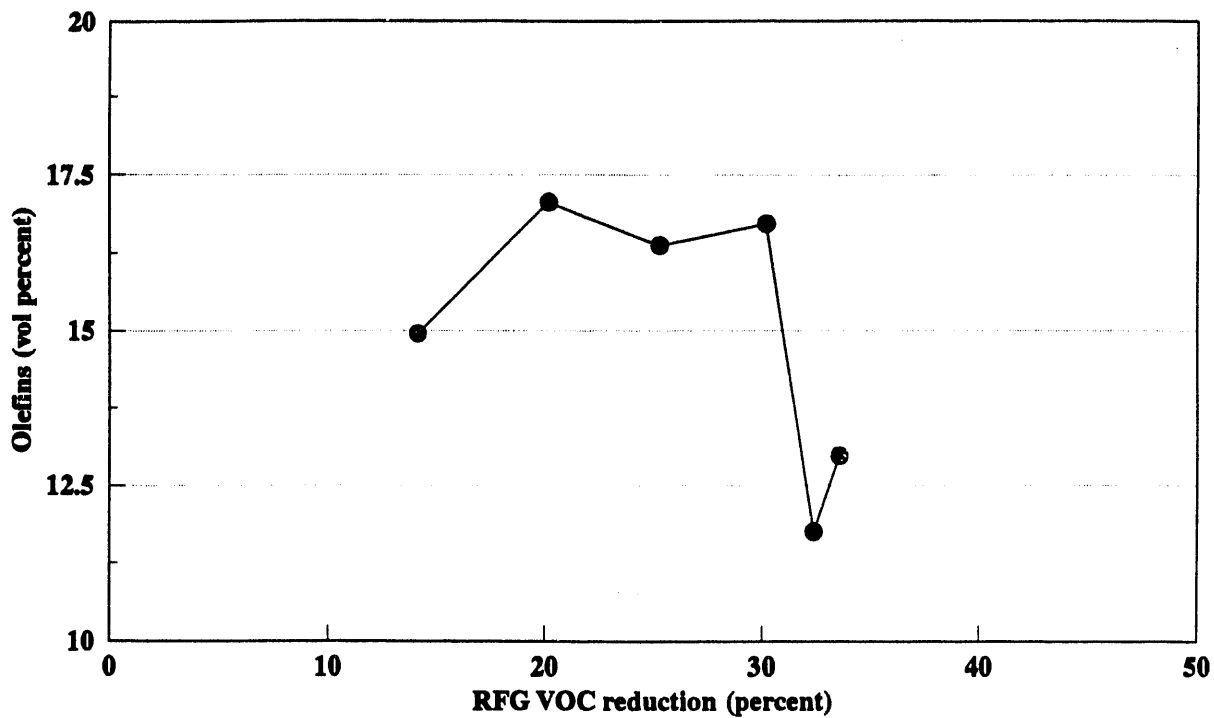


Fig. 4.8.
PADD I RFG benzene versus VOC reduction

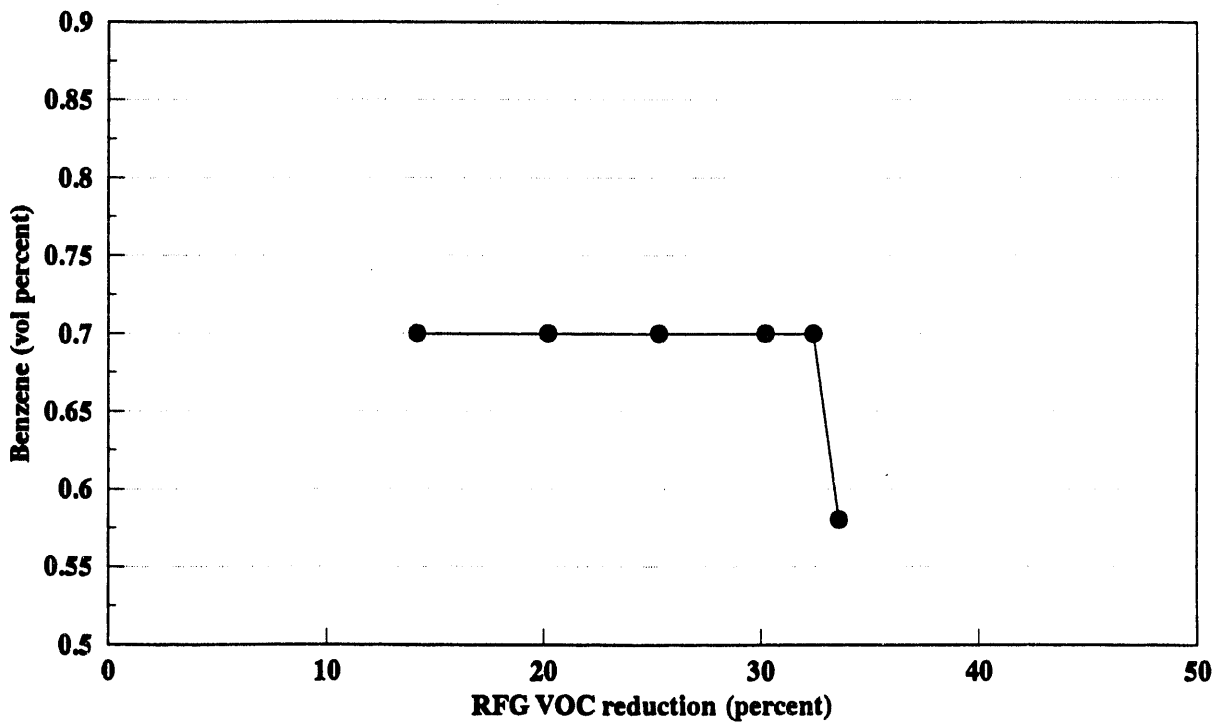


Fig. 4.9.
PADD I RFG T90 versus VOC reduction

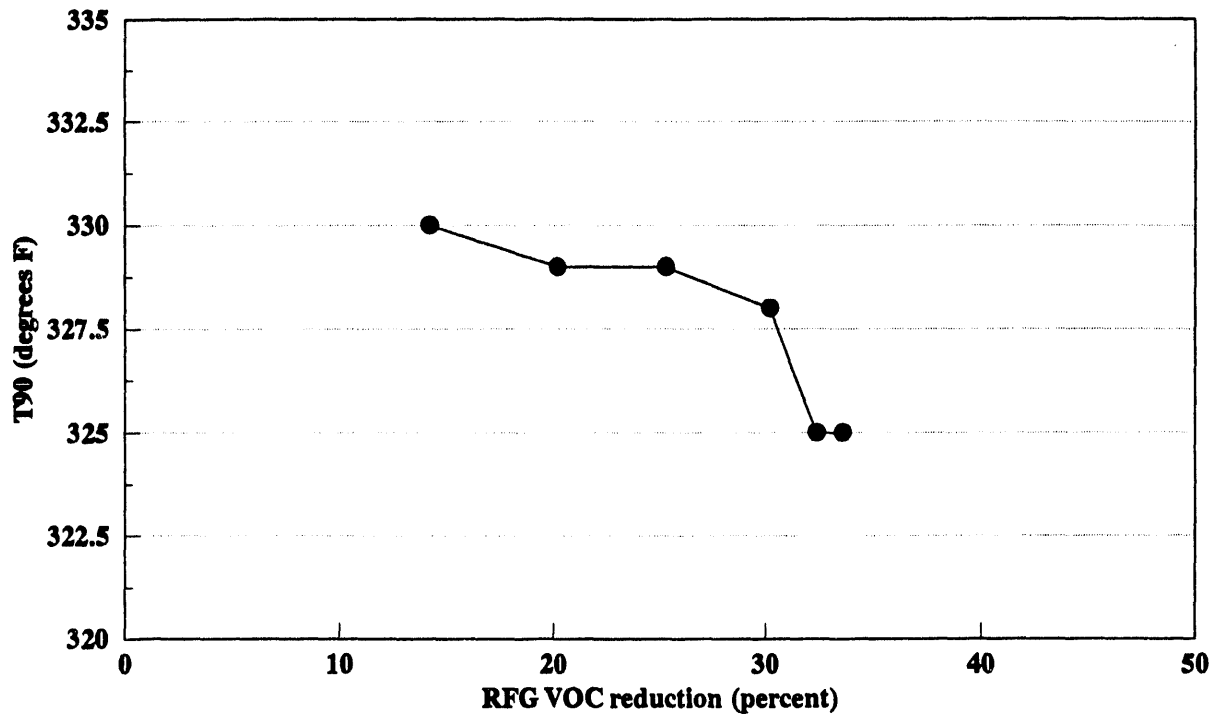
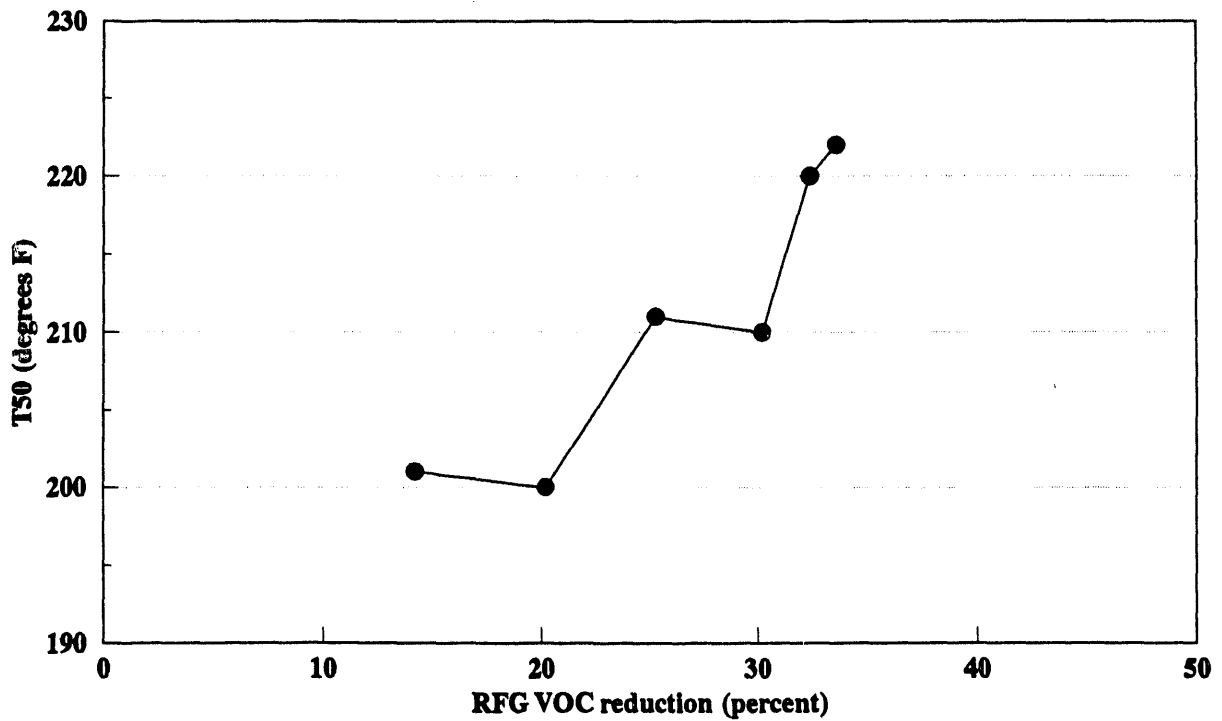


Fig. 4.10.
PADD I RFG T50 versus VOC reduction



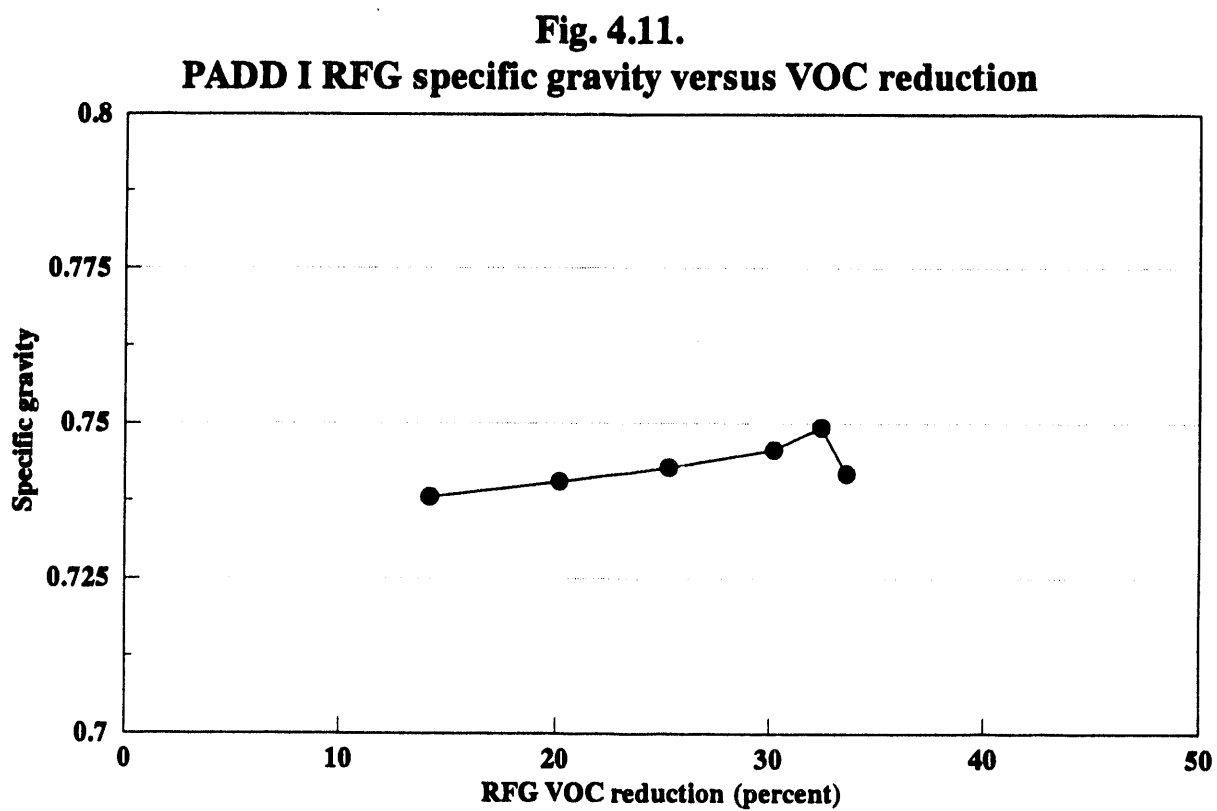


Fig. 4.12.
PADD III reformulation cost versus VOC reduction

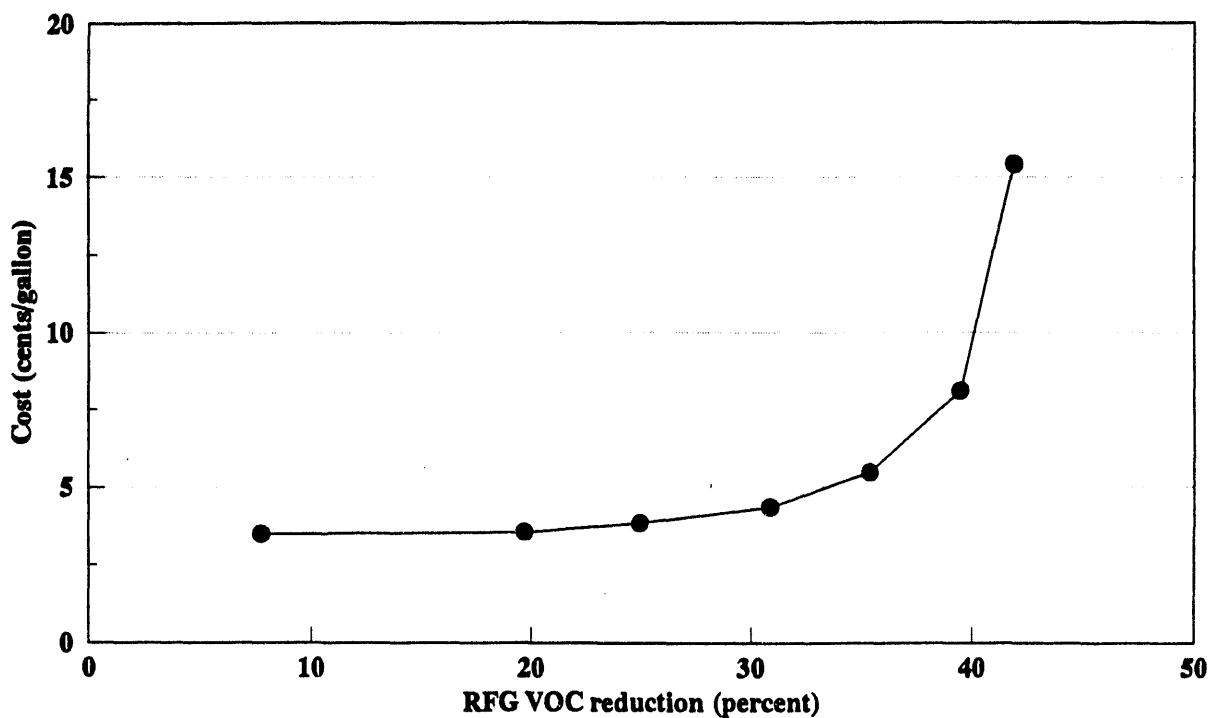


Fig. 4.13.
PADD III gasoline VOC versus VOC reduction

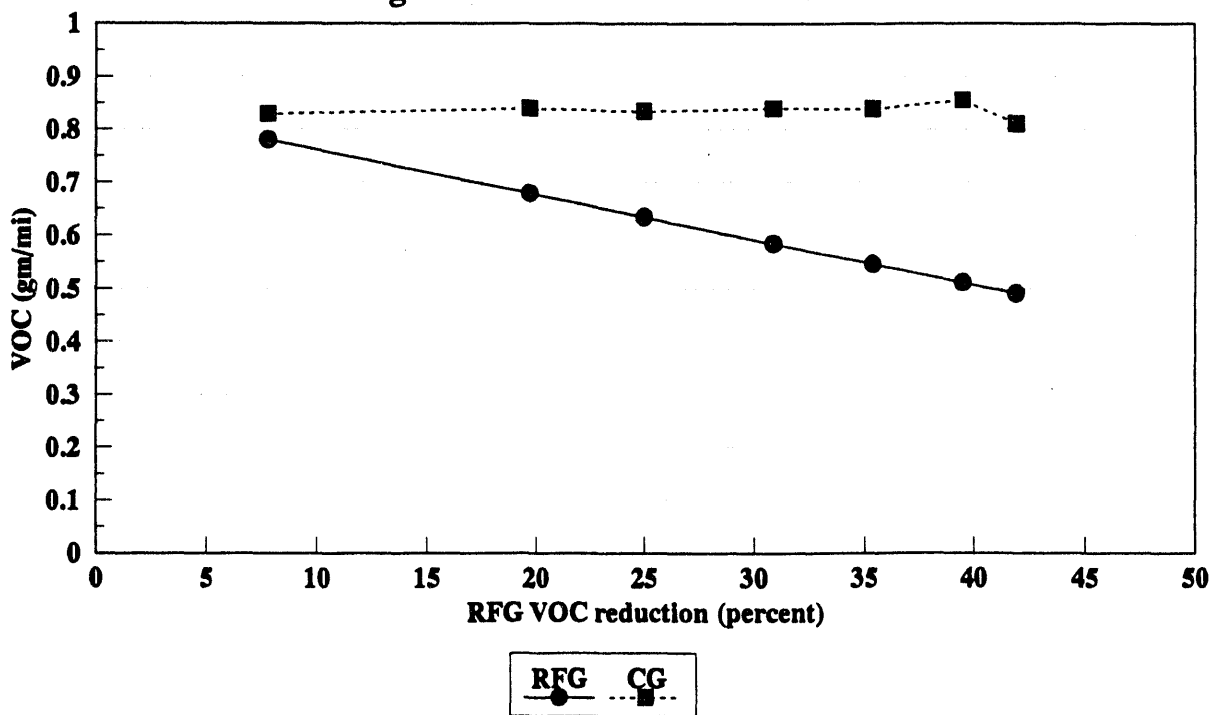


Fig. 4.14.
PADD III gasoline NOX versus VOC reduction

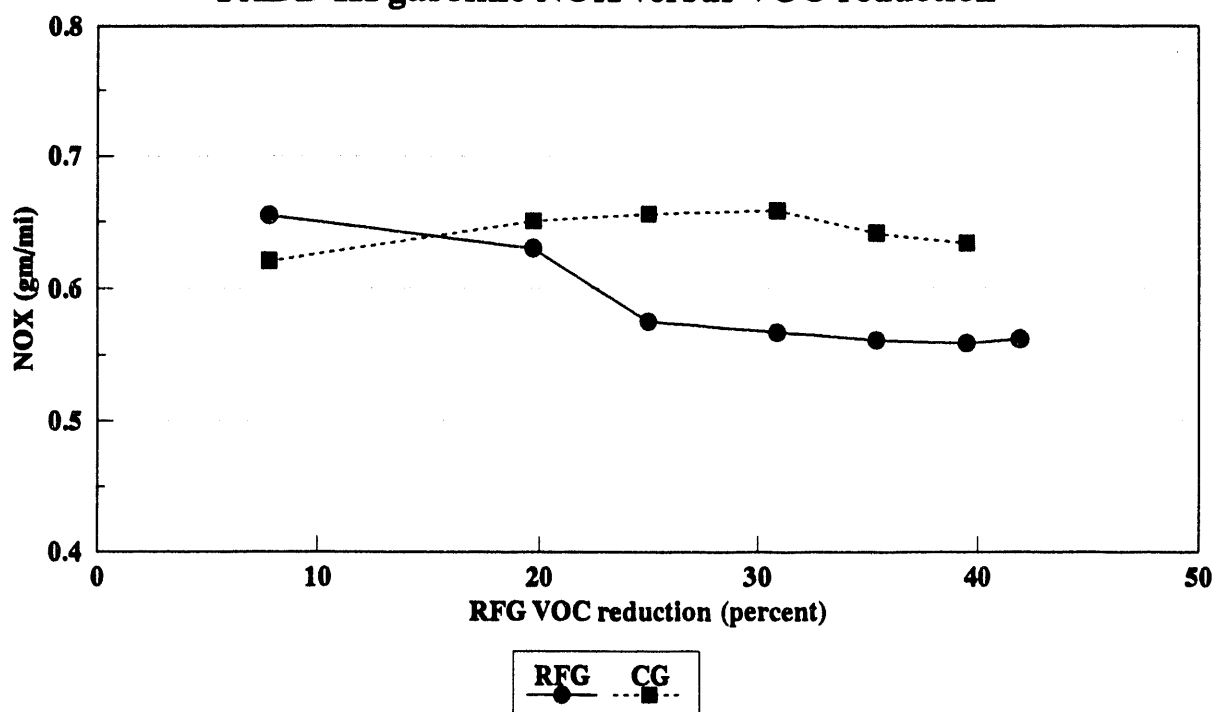


Fig. 4.15.
PADD III gasoline TAP versus VOC reduction

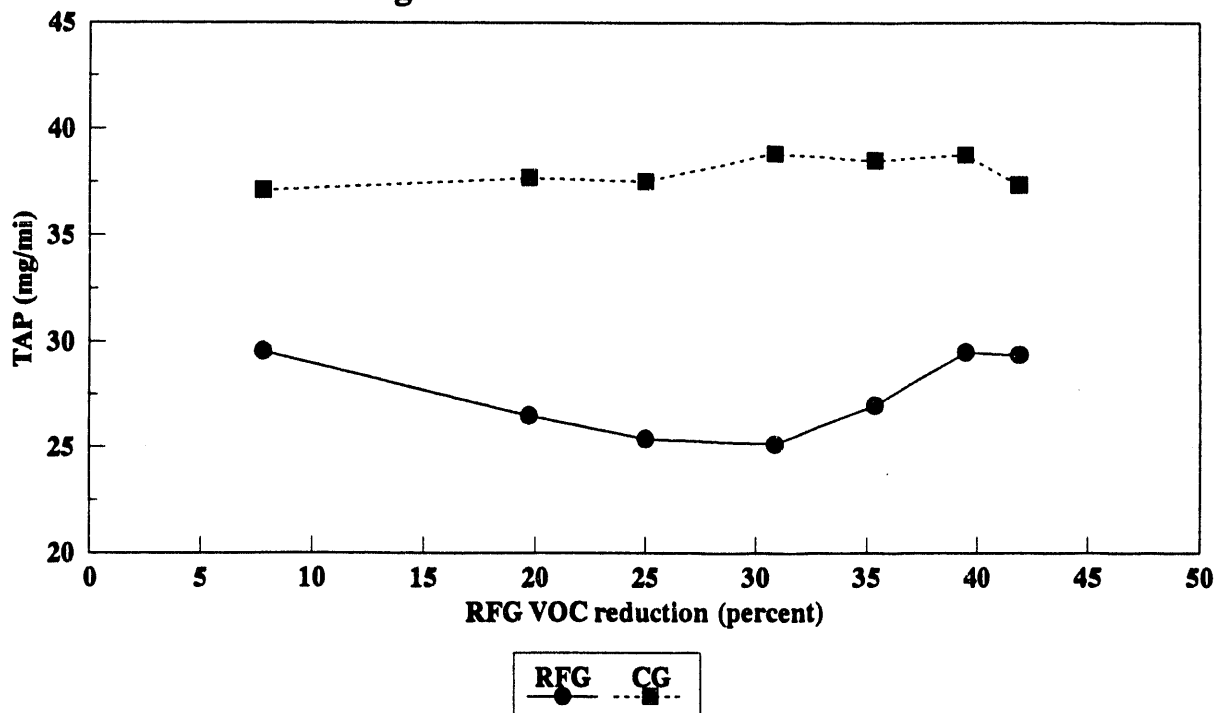


Fig. 4.16.
PADD III gasoline RVP versus VOC reduction

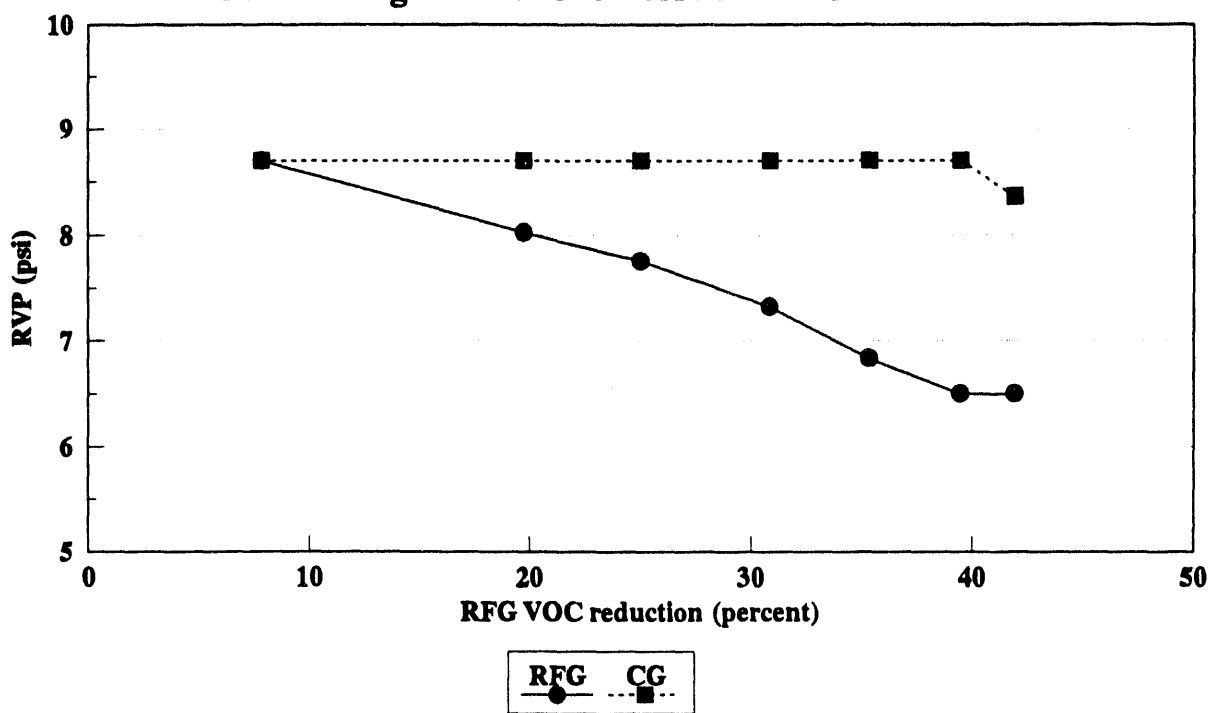


Fig. 4.17.
PADD III gasoline aromatics versus VOC reduction

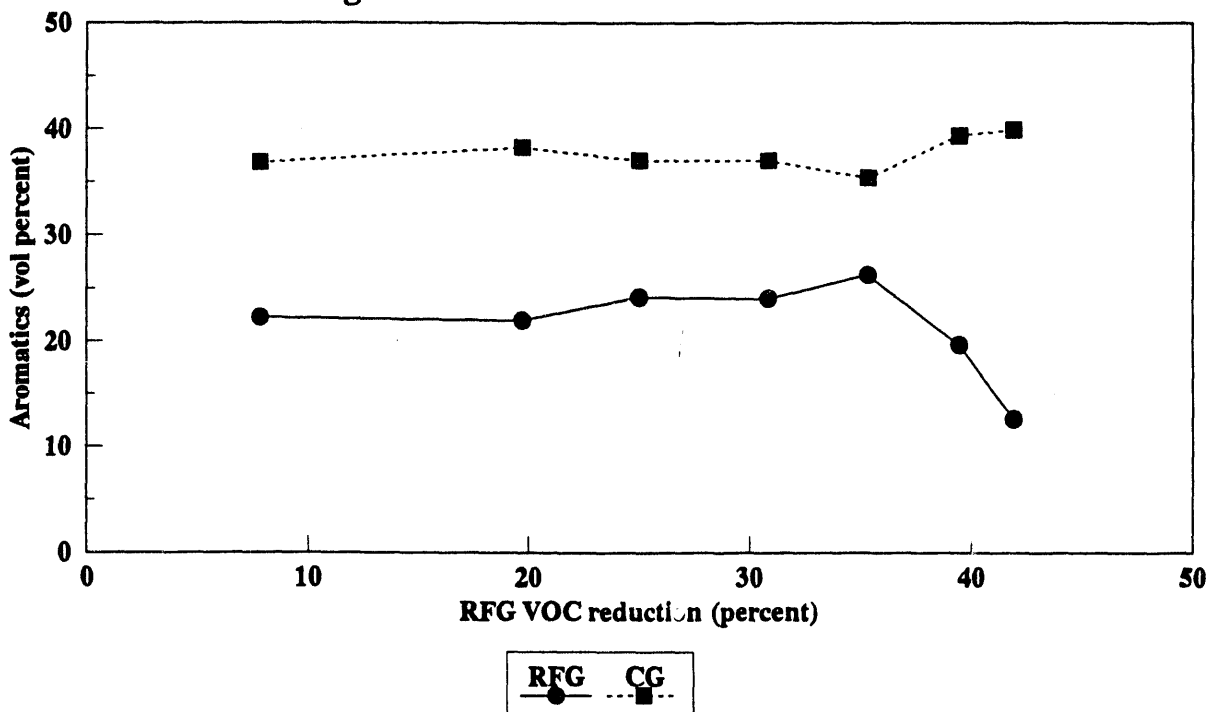


Fig. 4.18.
PADD III gasoline sulfur versus VOC reduction

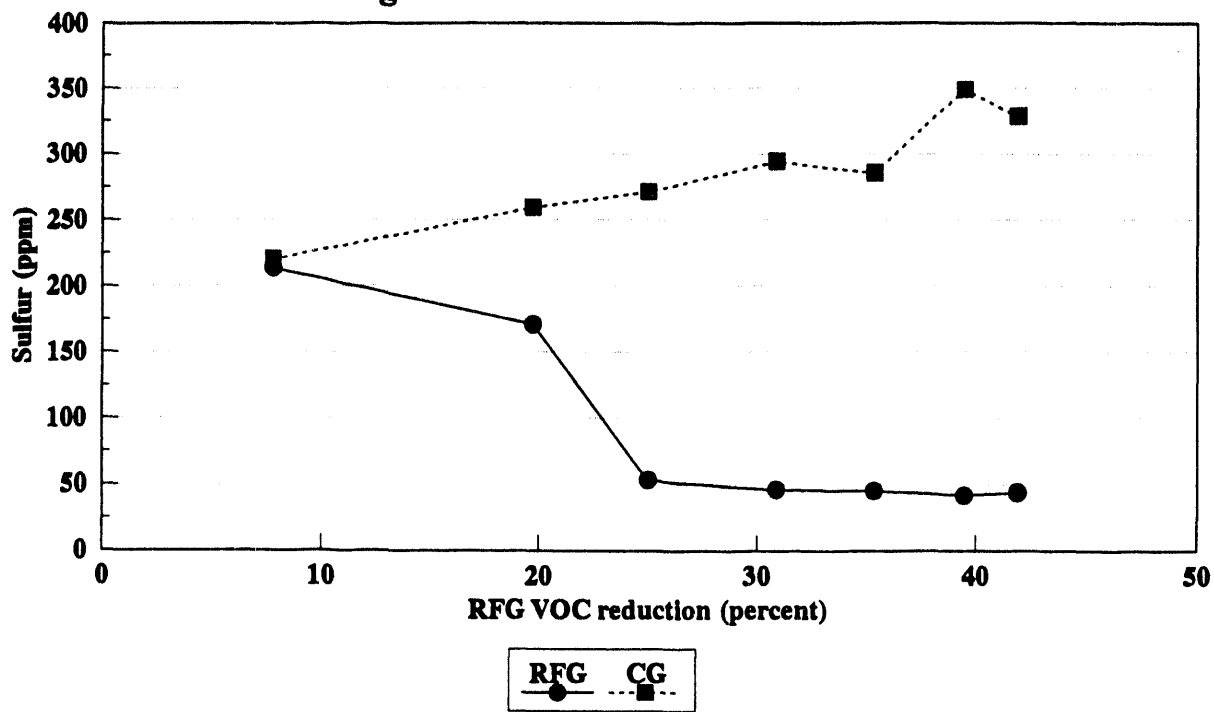


Fig. 4.19.
PADD III gasoline olefins versus VOC reduction

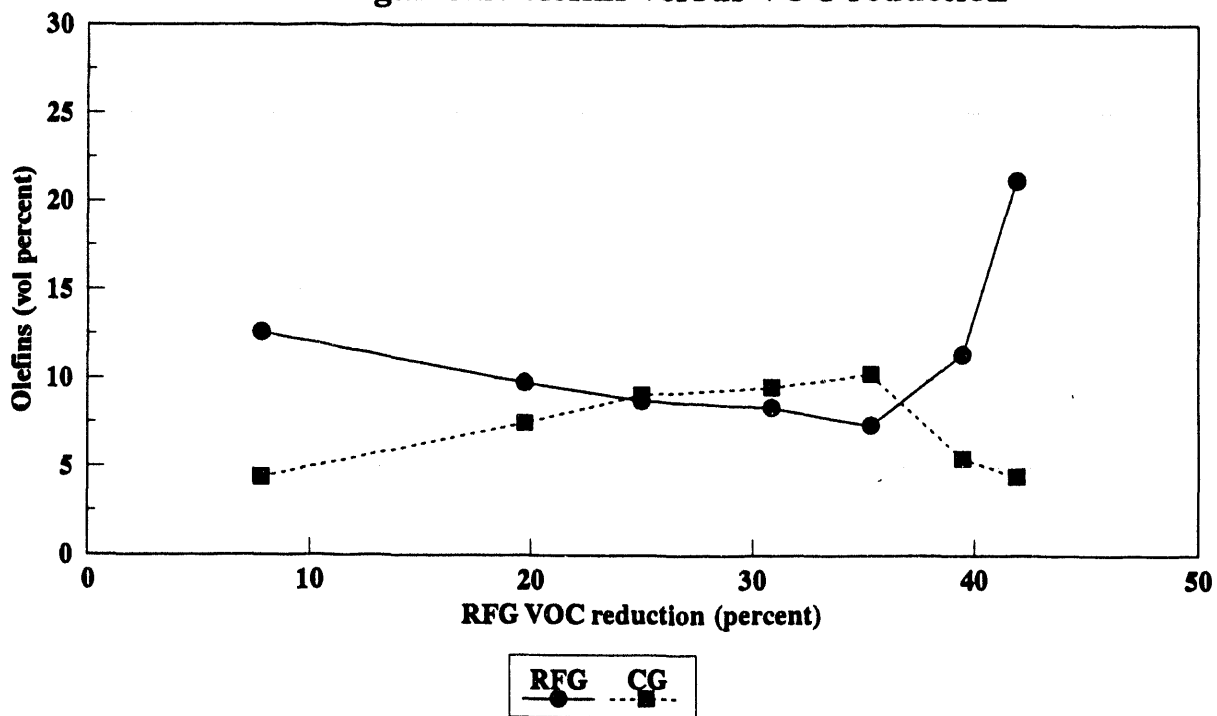


Fig. 4.20.
PADD III gasoline benzene versus VOC reduction

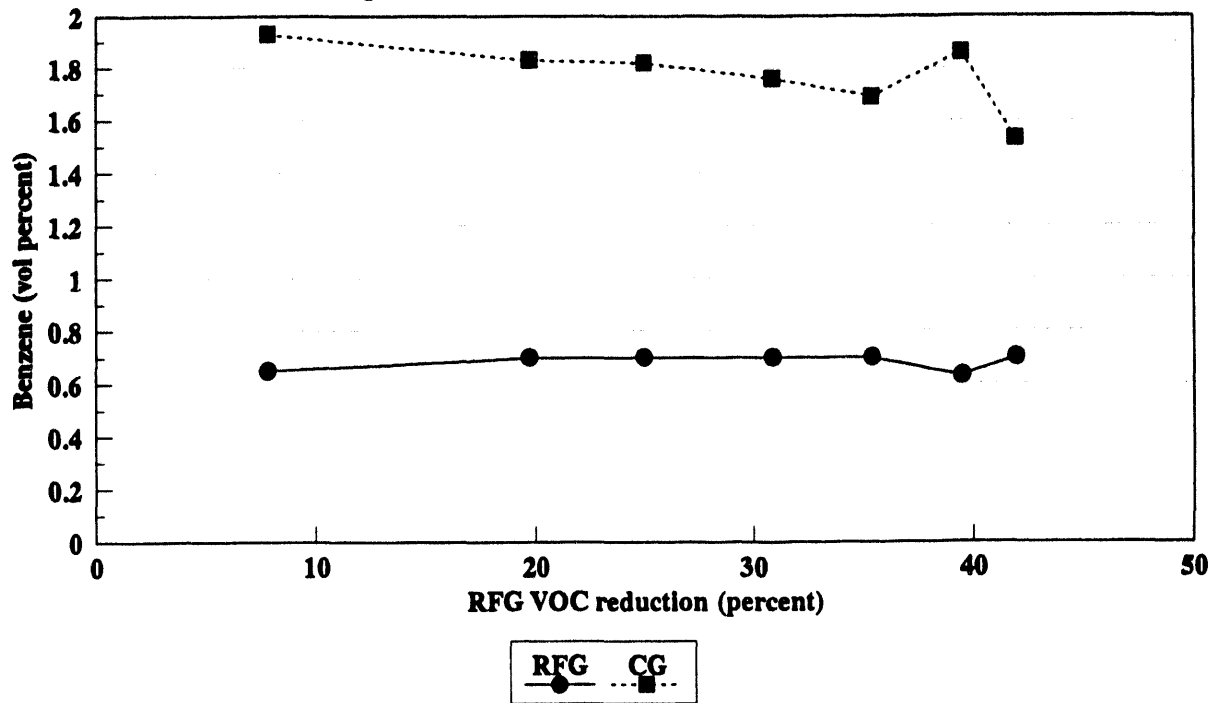


Fig. 4.21.
PADD III gasoline T90 versus VOC reduction

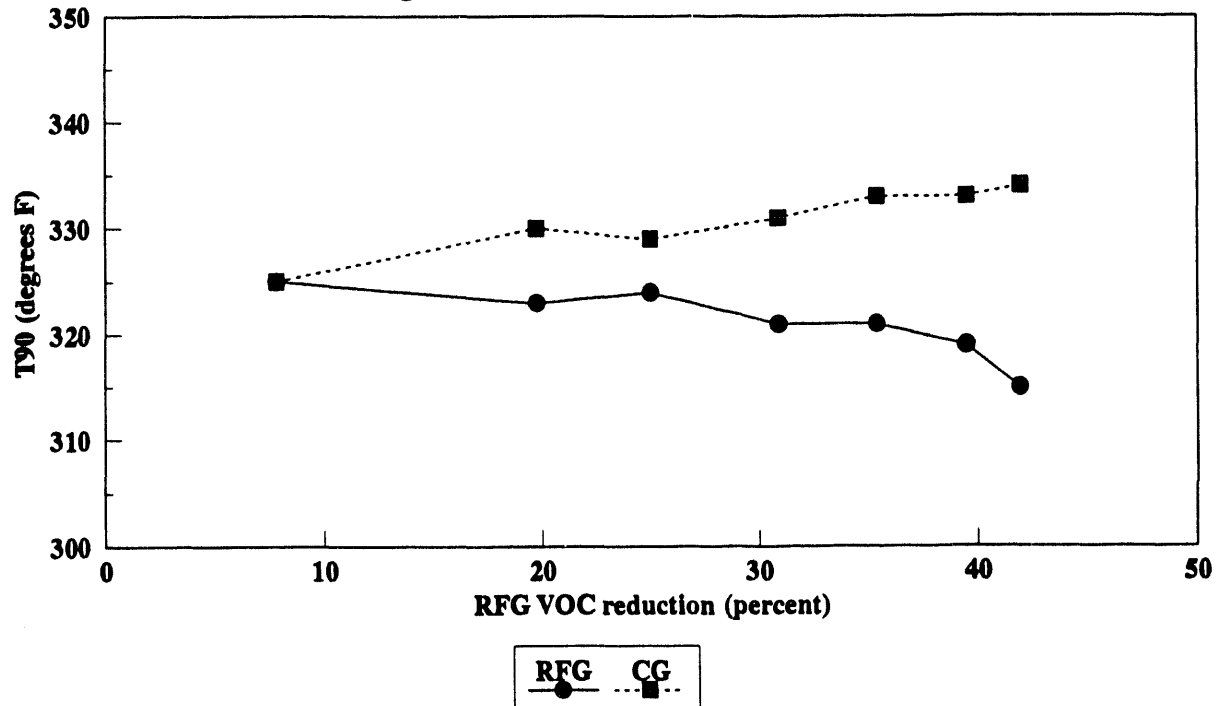


Fig. 4.22.
PADD III gasoline T50 versus VOC reduction

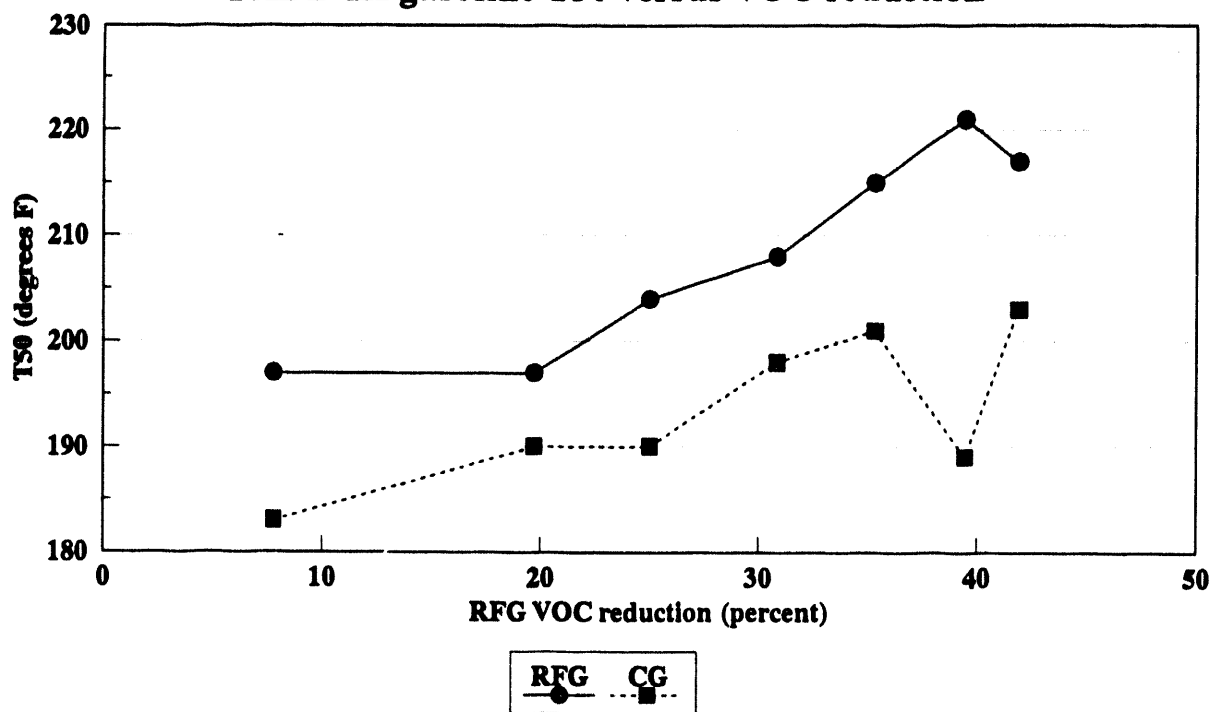
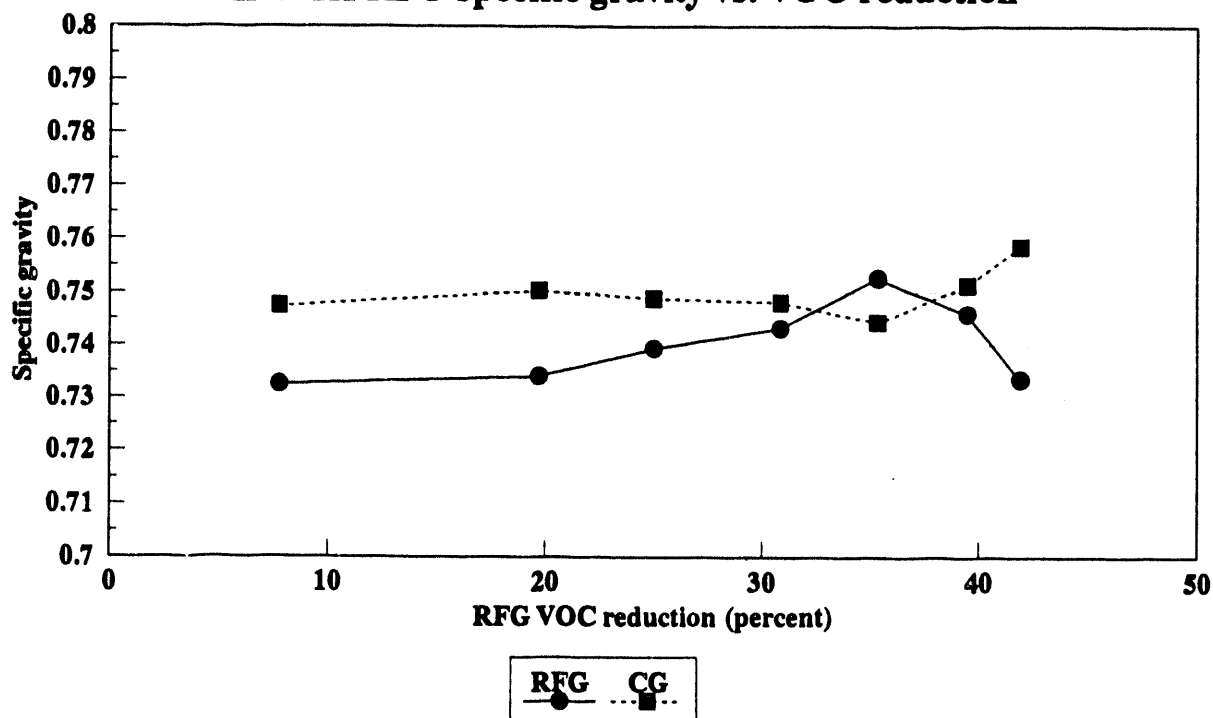


Fig. 4.23.
PADD III RFG specific gravity vs. VOC reduction



5. EMISSION MODEL EFFECTS

In addition to models already cited, several other emissions models have been estimated. For example, in October 1992, the American Petroleum Institute (API) presented the exhaust nonmethane hydrocarbon emissions model and NOX model shown in Tables 5.1 and 5.2.²¹

Table 5.1.
Exhaust nonmethane hydrocarbon (NMHC) model
of
American Petroleum Institute
(October 22, 1992)²¹

$$\begin{aligned} \text{NMHC(i)} = & 0.43/\text{Predicted Value for Industry Average Fuel x} \\ & \exp [\text{Intercept} \\ & + 0.00237449 \times (\text{aromatics}-28.0661) \\ & - 0.00290282 \times (\text{olefins}-6.8364) \\ & + 0.000470891 \times (\text{sulfur}-198.0640) \\ & + 0.0401532 \times (\text{RVP}-8.7741) \\ & + 0.00266509 \times (\text{T50}-207.0125) \\ & + 0.00151747 \times (\text{T90}-311.9345) \\ & - 0.00323241 \times (\text{oxygen}-1.2045) \\ & + 0.00084067 \times (\text{aromatics}-28.0661) \times (\text{oxygen}-1.2045) \\ & + 0.00006213 \times (\text{aromatics}-28.0661) \times (\text{T90}-311.9345) \\ & + 0.00005759 \times (\text{T50}-207.0125) \times (\text{T50}-207.0125) \\ & + 0.00001431 \times (\text{T90}-311.9345) \times (\text{T90}-311.9345) \\ & - 0.00762273 \times (\text{oxygen}-1.2045) \times (\text{oxygen}-1.2045) \\ & - 0.00000076 \times (\text{sulfur}-198.0640) \times (\text{sulfur}-198.0640)] \end{aligned}$$

VOC Exhaust (gm/mi) approximately =
baseline known mass x NMHC(i)/NMHC(baseline)

VOC Exhaust approximately = 0.41683 x NMHC(i)/1.1189

Table 5.2.
NOX model of American Petroleum Institute
(October 22, 1992)²¹

$$N(i) = 1/\text{Predicted Value for Industry Average Fuel x} \\ \exp [\text{Intercept} \\ + 0.000480167 \times (\text{aromatics}-28.0661) \\ + 0.0038605 \times (\text{olefins}-6.8364) \\ + 0.000518755 \times (\text{sulfur}-198.0640) \\ + 0.0104628 \times (\text{RVP}-8.7741) \\ - 0.000039167 \times (\text{T50}-207.0125) \\ - 0.00055664 \times (\text{T90}-311.9345) \\ + 0.00879458 \times (\text{oxygen}-1.2045) \\ - 0.0013696 \times (\text{aromatics}-28.0661) \times (\text{oxygen}-1.2045) \\ - 0.000054670 \times (\text{aromatics}-28.0661) \times (\text{T50}-207.0125) \\ - 0.00000856 \times (\text{T90}-311.9345) \times (\text{T90}-311.9345) \\ - 0.00000179 \times (\text{sulfur}-198.0640) \times (\text{sulfur}-198.0640)]$$

$$\text{NOX (gm/mi)} = \text{baseline known mass} \times N(i)/N(\text{baseline})$$

$$\text{NOX (gm/mi)} = 0.65999 \times N(i)/1.02845$$

For the PADD I and PADD III RFGs discussed in Section 4, Tables 5.3 and 5.4 compare total VOC and NOX emissions estimated with three sets of models:

EPA: the VOC and NOX models published by EPA in October 1992 (see Appendix A).¹³

DOE: (1) the non-linear exhaust VOC model B1¹¹ and the non-linear NOX model D1 of ACCA;¹² and (2) non-exhaust VOC model published by EPA in October 1992.¹³

API: (1) the non-linear exhaust nonmethane hydrocarbon model and the non-linear NOX model presented by API on October 22, 1992;²¹ and (2) non-exhaust VOC model published by EPA in October 1992.¹³

Table 5.3.
Emissions comparisons for PADD 1 RFGs
(Shaded cells indicate RFGs with olefins content > 9.2 percent)

Study RFG observation number	Emission	Percent reduction by model:		
		EPA	DOE	API
#1	Total VOC	10	14	15
	NOX	4	7	7
#2	Total VOC	13	20	21
	NOX	2	10	10
#3	Total VOC	19	25	26
	NOX	-2	11	11
#4	Total VOC	24	30	31
	NOX	-7	12	11
#5	Total VOC	32	32	33
	NOX	-2	13	12
#6	Total VOC	33	34	35
	NOX	-8	14	12

Table 5.4. Emissions comparisons for PADD III RFGs (Shaded cells indicate RFGs with olefins content > 9.2 percent)				
Study RFG observation number	Emission	Percent reduction by model:		
		EPA	DOE	API
#1	Total VOC	8	8	7
	NOX	6	1	0
#2	Total VOC	21	20	20
	NOX	9	5	4
#3	Total VOC	25	25	25
	NOX	13	13	13
#4	Total VOC	31	31	31
	NOX	12	14	14
#5	Total VOC	36	35	36
	NOX	10	15	15
#6	Total VOC	40	40	40
	NOX	-1	15	13
#7	Total VOC	32	42	43
	NOX	-48	15	9

Tables 5.3 and 5.4 show generally good agreement between the DOE and API models. However, most of the DOE and API model NOX values are considerably different from the EPA model NOX values. Figs. 5.1 and 5.2, developed by ACCA, demonstrate why the DOE and EPA NOX models produce different results in the ORNL-RYM studies. Recall that RVP reduction is a dominant VOC reduction mechanism. Fig. 5.1 shows that for a given olefins content, *RVP reduction reduces NOX* in the DOE NOX model.

However, as shown in Fig. 5.2 for the EPA NOX model, *RVP reduction increases NOX* for gasolines with olefins content greater than 9.2 percent. In Tables 5.3 and 5.4, the NOX cells are shaded for those gasoline with olefins contents greater than 9.2 percent. For example, PADD III RFG #7 has an olefins content of 21 percent and an RVP of 6.5 psi. The EPA model NOX emission of PADD III RFG #7 is 0.98 gm/mi, but the DOE model NOX emission is only 0.56 gm/mi.

Tables 5.3 and 5.4 show that all study RFGs are NOX-compliant, given the DOE and API emissions models. However, half the study RFGs are not in compliance with EPA-derived NOX standards.

Fig. 5.1.
DOE (ACCA) model effect of olefins on NOX
for various RVPs

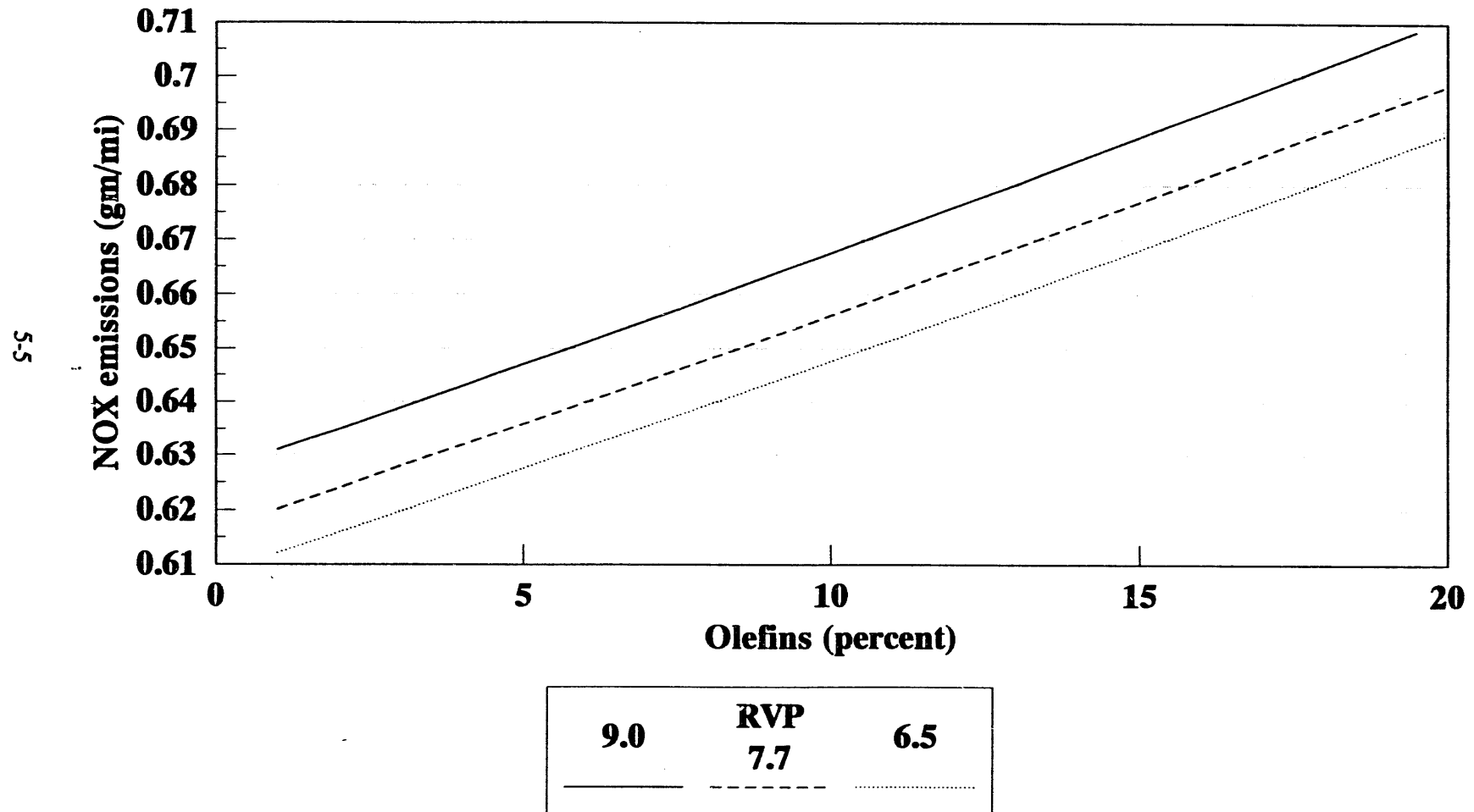
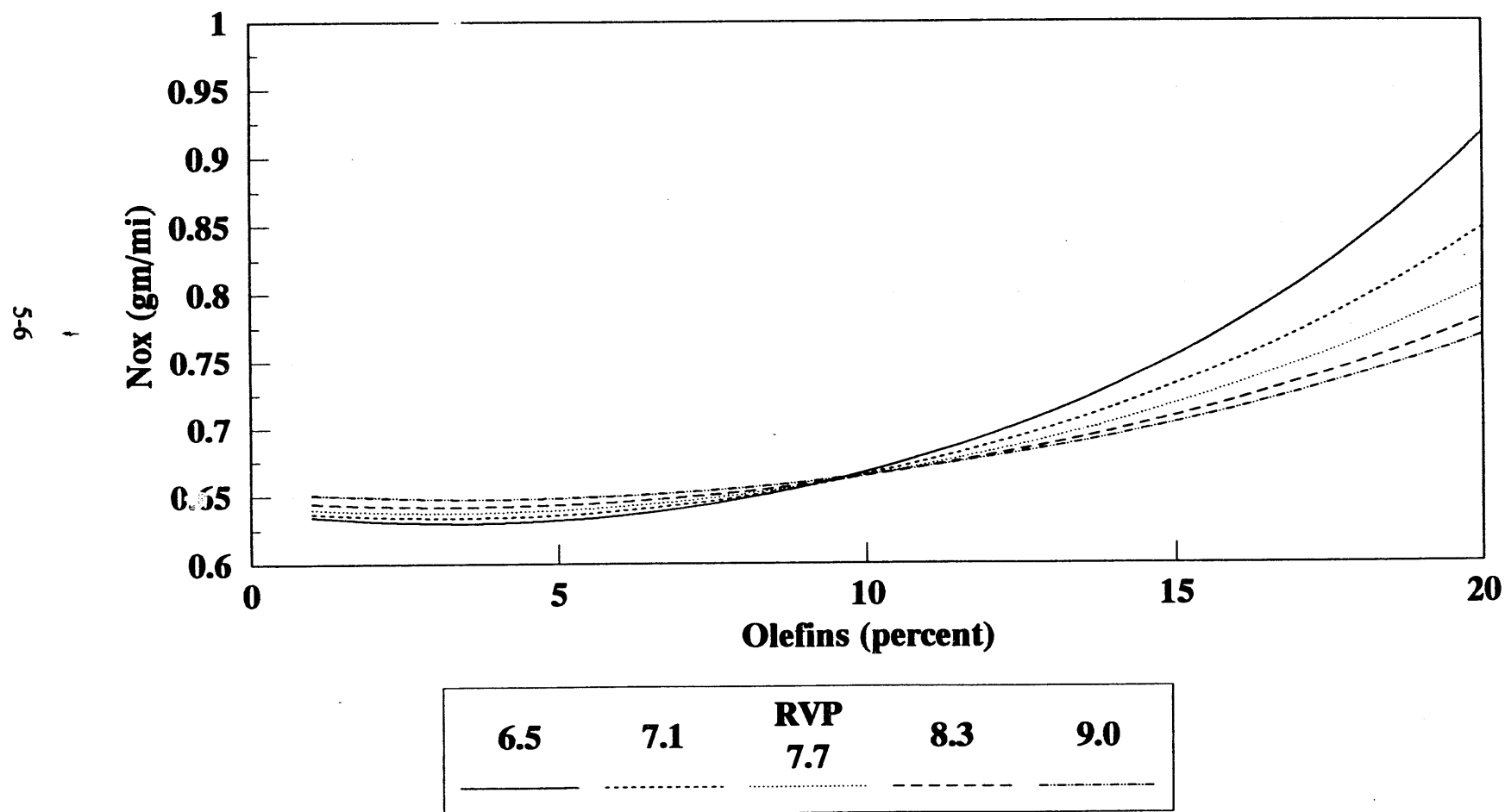


Fig. 5.2.
EPA model effect of olefins on NOX
for various RVPs



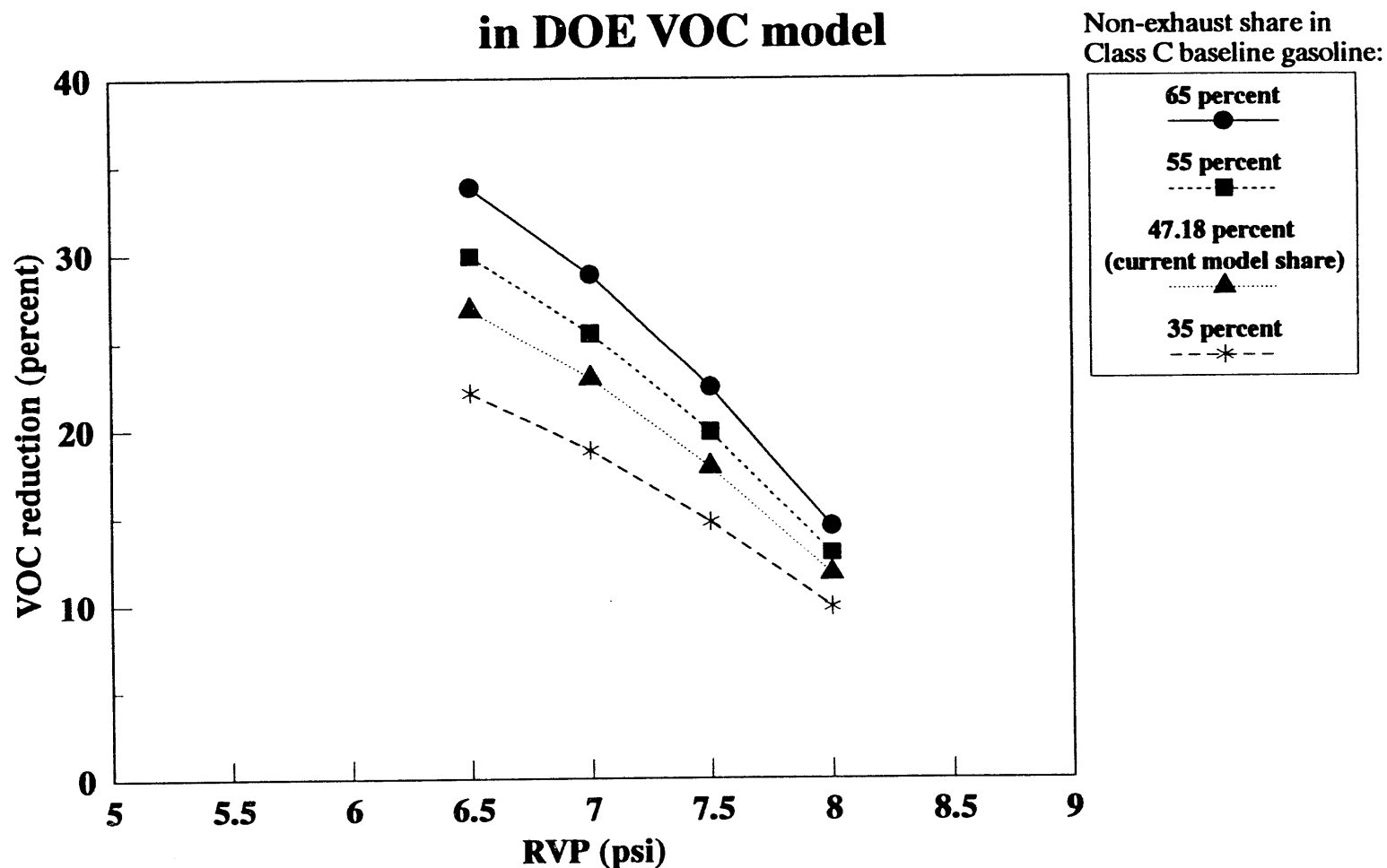
6. OTHER RFG PRODUCTION SENSITIVITIES

In addition to the potentially large *sensitivity of RFG production to different emissions models*, *RFG production is sensitive to the non-exhaust VOC share assumption* for a particular VOC model. Non-exhaust VOC is a function of RVP alone, and RVP reduction is a dominant VOC reduction mechanism. Fig. 6.1 shows that the non-exhaust VOC share assumption could have a large effect on VOC reduction, and therefore a large effect on the cost of reformulation. For example, in the 6.5 psi RVP RFGs of Fig. 6.1, the total VOC reduction is increased from 27 percent to 34 percent by increasing the VOC share from 47 percent (the current level) to 65 percent in Class C areas.²²

ORNL-RYM was used to explore *VOC reduction cost sensitivity to the cost of capital*. For an average Texas Gulf Coast refinery producing 100 percent RFG at the VOC cost knee, an increase in the annual capital charge from 21 percent to 24.2 percent resulted in a 1.3 cents per gallon increase in the cost of reformulation.²³ The 21 percent capital charge corresponds to a 12.8 percent discounted cash flow return on investment (DCF ROI); the 24.2 percent capital charge corresponds to a 15 percent DCF ROI. ORNL-RYM uses an annual capital charge of 24.2 percent.

The *cost of RFG is sensitive to the RVP of CG*. In an analysis of an average Texas Gulf Coast refinery producing 50 percent RFG and 50 percent CG, ORNL-RYM estimated that RFG could cost 1 cent per gallon more when CG RVP is 7.8 psi compared to the cost of RFG when CG RVP is 9 psi.^{24,25}

Fig. 6.1.
Effect of non-exhaust share assumption
in DOE VOC model



Notes: 1) Exhaust VOC is 0.41682 gm/mi and RVP is 8.7 psi in each baseline gasoline.

2) Only RVP varies in graph. Aromatics = 25 percent; oxygen content = 2.1 percent; T90 = 330 degrees F; T50 = 218 degrees F; sulfur = 339 ppm.

7. COMPARISONS OF REFINING STUDIES

Policy makers may use the reformulation cost knee to set emissions reduction targets, giving due consideration to the differences between model representations and actual refining operations. ORNL-RYM estimates that the reformulation cost knee for PADD I is about 15.2 cents per gallon with a VOC reduction of 30 percent; and the estimated cost knee for PADD III is about 5.5 cents per gallon with a VOC reduction of 35 percent.

Reformulation cost estimates of various studies are compared in Table 7.1. These estimates range from about 5 to 15 cents per gallon. The studies are based upon different premises and assumptions about RFG specifications, and the cost estimates could be referenced to different baselines. In addition to the cost estimates of Table 7.1, a 1991 poll of industry executives suggested that the CAAA could increase the cost of refining gasoline enough to boost prices by 6 to 10 cents per gallon.³⁴

Table 7.1. Comparison of projected gasoline reformulation costs				
Source	Gasoline reformulation cost (cents/gal)	RFG share of total gasoline (%)	RFG RVP (psi)	RFG aromatics (vol %)
ORNL - Phase I RFG ^{26,27,28}	5.2 - 6.8 (PADD III); 5.7 (PADD I); 7.6 (PADD V)	50	7.0	25
EnSys ²⁹	5.5 - 7.5	100: switch from low volatility CG to RFG in typical U.S. deep-conversion refinery	8.5	20
ORNL - this report	5.5 (at PADD III cost knee)	50	6.8	23
	15.2 (at PADD I cost knee)	100	7.1	26
Turner, Mason and Company (TMC) ³⁰	7-11 (average U.S.)	Opt-in of all non- attainment areas	Varies	Varies
EPA ³¹	8.2-12.0 (marginal refining costs for cost effectiveness < \$5,000 per ton + mpg cost of effect of 1.72-1.76 cents per gallon)			
Wright Killen & Co. ³²	10.2	100: switch to RFG in high conversion refinery with no BTX production	9.0 (base case gasoline RVP is 10 psi)	25
Ashland Oil, Inc. ³³	10 - 15	80		

Premises for the ORNL studies in Section 4 of this report are similar to premises used in recent studies performed by Turner, Mason & Company (TMC) for the National Petroleum Council's Product Quality Task Group.³⁵ Tables 7.2 through 7.6 compare ORNL and TMC results for RFGs with similar VOC emissions reductions.

For the selected PADD I RFG, Tables 7.2 through 7.4 show similarities in reformulation costs and in the percentages of the major blendstocks (reformate and FCC naphtha). The ORNL and TMC capacity additions of Table 7.4 are quite different, due in part to the fact that ORNL-RYM does not have a representation of reformer feed fractionation to remove benzene precursors.

For the selected PADD III RFG in Tables 7.5 through 7.7, there is a premise difference in the RFG production share (50 percent for ORNL versus 63 percent for TMC). The ORNL and TMC percentages of reformate and FCC naphtha are quite different. Capacity additions are different, most notably for reformer feed fractionation.

Table 7.2. PADD I RFG comparison		
Attribute	TMC S10	ORNL #4
RFG production share, percent	100	100
Reformulation cost, cents per gallon	>13.1	15.2 [*]
(R+M)/2	88.9	89.6
Aromatics, vol percent	27.0	23.2
Ethers, vol percent	11.7	11.6
Oxygen, wt percent	2.1	2.1
Olefins, vol percent	10.2	16.7
Benzene, vol percent	0.7	0.7
Sulfur, ppm	30	58
RVP, psi	6.7	7.1
T50, °F	205	210
T90, °F	346	328
Specific gravity	0.7461	0.7457
VOC reduction, percent ^{**}	31	30
NOX reduction, percent ^{**}	16	12
TAP reduction percent ^{**}	28	25

^{*}Reformulation cost is relative to a baseline case with 100 percent CG with 8.7 psi RVP

^{**}Emissions are calculated with DOE model.

Table 7.3. PADD I RFG blendstock comparison (percent)		
Blendstock	TMC S10	ORNL #4
Butane	2.1	2.0
Reformate	25.9	24.8
Straight run naphtha	3.0	0.9
C5+ isomerate	4.6	5.3
FCC naphtha	31.8	33.8
Coker naphtha		
Hydrocrackate	2.4	0.8
Alkylate	10.8	14.5
Polymer gasolines	0.5	
Dimate		3.9
MTBE	11.2	6.5
Toluene/xylene		
Natural gasoline		
Pyrolysis gasoline		
Raffinates	6.6	
Other	1.1	7.6

Table 7.4. PADD I refinery capacity additions (MBD)		
Process	TMC S10	ORNL #4
FCC gasoline splitter	143	61
FCC gasoline fractionation	91	158
Coker gasoline splitter	2	
Reformer feed fractionation	289	
Reformate fractionation	67	
Benzene saturation	38	
Gasoline selective desulfurization	88	
Ether plant	4	57
C5/C6 isomerization	4	25
Hydrogen, MMSCF/PSD	4	1
C4 rerun - saturates	36	
C4 rerun - unsaturates	63	
Butene isomerization		36
Alkylation		19
Distillate deep hydrotreating		9
FCC feed hydrofiner		180
Naphtha cracker		51
Hydrocracker		12
C2/C5 dehydrogenation		26
Dimersol		26
C4 isomerization		9
Visbreaker		9

Table 7.5. PADD III RFG comparison		
Attribute	TMC Q6	ORNL #5
RFG production share, percent	63	50
Reformulation cost, cents per gallon	8.2	5.5*
(R+M)/2	88.6	89.2
Aromatics, vol percent	24.7	26.2
Ethers, vol percent	11.7	11.6
Oxygen, wt percent	2.1	2.1
Olefins, vol percent	11.6	7.4
Benzene, vol percent	0.7	0.7
Sulfur, ppm	144	45
RVP, psi	6.5	6.8
T50, °F	205	215
T90, °F	344	321
Specific gravity	0.7463	0.7526
VOC reduction, percent**	36	35
NOX reduction, percent**	8	15
TAP reduction, percent**	25	34

*Reformulation cost is relative to a baseline case with 100 percent CG with 8.7 psi RVP

**Emissions are calculated with DOE model.

Table 7.6. PADD III RFG blendstock comparison (percent)		
Blendstock	TMC Q6	ORNL #5
Butane	2.0	2.0
Reformate	21.9	38.7
Straight run naphtha	1.8	1.8
C5+ isomerate	5.1	6.0
FCC naphtha	32.2	16.9
Coker naphtha	0.7	
Hydrocrackate	2.1	5.2
Alkylate	13.3	15.1
Polymer gasolines	0.9	2.0
Dimate		0.2
MTBE	10.8	11.5
Toluene/xylene		
Natural gasoline		
Pyrolysis gasoline		
Raffinates	7.3	0.5
Other	1.9	0.2

Table 7.7. PADD III refinery capacity additions (MBD)		
Process	TMC Q6	ORNL #5
FCC gasoline splitter	726	61
Coker gasoline splitter	25	
Reformer feed fractionation	1,497	
Reformate fractionation	258	
Benzene saturation	64	
Ether plant	27	37
Butene isomerization for alkylation		128

8. CONCLUSIONS

Studies of RFG costs and refinery impacts have been performed with ORNL-RYM, a linear program which has been updated to blend gasolines to satisfy emissions constraints defined by preliminary complex emissions models. Study findings include the following:

The reformulation cost knee for PADD I is about 15.2 cents per gallon with a 30 percent reduction of VOCs; and the estimated cost knee for PADD III is about 5.5 cents per gallon with a VOC reduction of 35 percent. Policy makers may use the reformulation cost knee to set emissions reduction targets, giving due consideration to the differences between model representations and actual refining operations. Reformulation cost estimates of various other studies range from about 5 to 15 cents per gallon. The studies are based upon different premises and assumptions about RFG specifications, and the cost estimates could be referenced to different baselines.

The dominant VOC reduction mechanism is RVP reduction.

Even with anti-dumping constraints, conventional gasoline appears to be an important sink which permits RFG to be blended with lower aromatics and sulfur contents in PADD III.

Refinery capacity additions, estimated by ORNL-RYM, for low-VOC RFG production in PADD I include FCC feed hydrofining, FCC gasoline fractionation, alkylation, ether production, and feed preparation for alkylation and etherification. Capacity additions in PADD III, estimated by ORNL-RYM, include FCC gasoline fractionation, ether production, and feed preparation for alkylation and dimersol/polymerization units. Other studies place substantially greater emphasis on investment in reformer feed fractionation to satisfy CAAA constraints for benzene in gasolines.

ORNL-RYM requires a representation of reformer feed fractionation. Benzene reduction for RFGs can be accomplished by removing benzene precursors from reformer feed. In refining situations with ample ethers for octane improvement, the removed material can be blended directly into gasoline.

The RFG production assumption of 100 percent could be high for PADD I, and 50 percent RFG could be low for PADD III. Estimated costs for 100 percent gasoline reformulation in PADD I are substantially greater than costs for 50 percent gasoline reformulation in PADD III. The likely production shares in PADDs I and III could be estimated, given regional curves of cost versus production share and given the inter-regional delivery costs.

Refinery analysis with EPA emissions equations could identify refining costs and problems unique to the EPA Complex Model. All RFGs of the PADD I and PADD III studies are NOX-compliant, given the DOE emissions models. However, half the study RFGs are not in compliance with EPA-derived NOX standards. A factor contributing to this discrepancy is that, with the EPA Complex Model of October 1992, RVP reduction increases NOX emissions for gasolines with olefins contents greater than 9.2 percent.

RFG production is sensitive to the non-exhaust VOC share assumption for a particular VOC model. ORNL-RYM has also been used to estimate the sensitivity of RFG production to the cost of capital; to the RVP requirements for conventional gasoline; and to the percentage of RFG produced in a refining region.

Complex non-linear emissions models can be represented in a refinery linear program by assuming that an emission value can be represented as a base emission value plus small linear emissions changes due to small changes in gasoline properties.

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Appendix A. EPA Complex Model

A.Complex Exhaust Emissions Model Equations

1.Exhaust VOC Emissions

EPA's analysis indicates that the fuel effects on exhaust VOC emissions can best be represented by the following equations, which EPA propose for use in certifying reformulated fuels:

$$\text{Exhaust VOC (grams/mile)} = \sum k_i W_i e^{V_i}$$

VALUES OF k_i AND W_i FOR TECHNOLOGY GROUPS WITHIN NORMAL AND HIGH EMITTERS - VOC

TECHNOLOGY GROUP	NORMAL EMITTERS		HIGH EMITTERS	
	k_i	W_i	k_i	W_i
1	0.243867	0.219562	1.083512	0.043922
2	0.218241	0.239684	0.706996	0.047948
3	0.209866	0.182016	0.517712	.036411
4	0.387476	0.100704	1.451855	0.020145
5	0.112358	0.036002	0.590040	0.007202
6	0.210686	0.000104	0	0
7	0.374647	0.043846	1.206235	0.008771
8	0	0	0	0
9	0.224201	0.013682	0	0

Technology Group 1--Normal Emitters

$$V_i = \{ [(-0.01131514) \times (X - 1.415043)] + [(0.00037348) \times (S - 163.0367287)] + [(0.07347939) \times (RVP - 8.8858423)] + [(0.00325939) \times (T50 - 205.153526)] + [(0.00247407) \times (T90 - 310.8900588)] + [(0.00440111) \times (A - 27.5484329)] + [(0.00355247) \times (O - 6.536288)] + [(0.0000489) \times (T50 - 205.153526)^2] + [(0.00017678) \times (A - 27.5484329)^2] +$$

$$\begin{aligned}
& [(0.00059373) \quad x \quad (X - 1.415043) x (T90 - 310.8900588)] + \\
& [(0.00227009) \quad x \quad (X - 1.415043) x (A - 27.5484329)] + \\
& [(-4.362 \times 10^{-5}) \quad x \quad (S - 163.0367287) x (O - 6.536288)] + \\
& [(0.00185642) \quad x \quad (RVP - 8.8858423) x (T50 - 205.153526)] + \\
& [(0.0000841) \quad x \quad (T50 - 205.153526) x (T90 - 310.8900588)] \}
\end{aligned}$$

Technology Group 2--Normal Emitters

$$\begin{aligned}
V_i = & \{ [(-0.006808) \quad x \quad (X - 1.415043)] + \\
& [(0.000111) \quad x \quad (S - 163.0367287)] + \\
& [(0.017033) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.002479) \quad x \quad (T50 - 205.153526)] + \\
& [(0.001966) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.002321) \quad x \quad (A - 27.5484329)] + \\
& [(0.008760) \quad x \quad (O - 6.536288)] + \\
& [(-9.29 \times 10^{-7}) \quad x \quad (S - 163.0367287)^2] + \\
& [(0.0005220) \quad x \quad (X - 1.415043) x (T90 - 310.8900588)] + \\
& [(0.0011870) \quad x \quad (X - 1.415043) x (O - 6.536288)] + \\
& [(-6.467 \times 10^{-5}) \quad x \quad (S - 163.0367287) x (O - 6.536288)] + \\
& [(0.00006854) \quad x \quad (T50 - 205.153526) x (T90 - 310.8900588)] + \\
& [(0.000187) \quad x \quad (T50 - 205.153526) x (A - 27.5484329)] + \\
& [(-5.7374 \times 10^{-5}) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] \}
\end{aligned}$$

Technology Group 3--Normal Emitters

$$\begin{aligned}
V_i = & \{ [(0.007589) \quad x \quad (X - 1.415043)] + \\
& [(0.000517) \quad x \quad (S - 163.0367287)] + \\
& [(0.057474) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.003964) \quad x \quad (T50 - 205.153526)] + \\
& [(0.000247) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.001756) \quad x \quad (A - 27.5484329)] + \\
& [(0.012813) \quad x \quad (O - 6.536288)] + \\
& [(-0.000255) \quad x \quad (A - 27.5484329)^2] + \\
& [(-0.000879) \quad x \quad (O - 6.536288)^2] + \\
& [(0.000139) \quad x \quad (X - 1.415043) x (S - 163.0367287)] + \\
& [(-0.000847) \quad x \quad (X - 1.415043) x (T50 - 205.153526)] + \\
& [(0.001536) \quad x \quad (X - 1.415043) x (T90 - 310.8900588)] + \\
& [(-5.9304 \times 10^{-5}) \quad x \quad (S - 163.0367287) x (O - 6.536288)] + \\
& [(0.000146) \quad x \quad (T50 - 205.153526) x (T90 - 310.8900588)] + \\
& [(0.000121) \quad x \quad (T90 - 310.8900588) x (A - 27.5484329)] + \\
& [(0.000205) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] \}
\end{aligned}$$

Technology Group 4--Normal Emitters

$$\begin{aligned}
V_i = & \{ [(-0.011963) \quad x \quad (X - 1.415043)] + \\
& [(0.001194) \quad x \quad (S - 163.0367287)] + \\
& [(-0.027223) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.001640) \quad x \quad (T50 - 205.153526)] + \\
& [(0.000931) \quad x \quad (T90 - 310.8900588)] +
\end{aligned}$$

$$\begin{aligned}
& [(-0.000515) \quad x \quad (A - 27.5484329)] + \\
& [(0.004589) \quad x \quad (O - 6.536288)] + \\
& [(0.011867) \quad x \quad (X - 1.415043)^2] + \\
& [(-3.721 \times 10^{-6}) \quad x \quad (S - 163.0367287)^2] + \\
& [(-0.000302) \quad x \quad (A - 27.5484329)^2] + \\
& [(-0.001866) \quad x \quad (X - 1.415043) \quad x \quad (A - 27.5484329)] + \\
& [(-2.3983 \times 10^{-5}) \quad x \quad (S - 163.0367287) \quad x \quad (A - 27.5484329)] + \\
& [(-9.275 \times 10^{-5}) \quad x \quad (S - 163.0367287) \quad x \quad (O - 6.536288)] + \\
& [(-0.002909) \quad x \quad (T50 - 205.153526) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.000095) \quad x \quad (T90 - 310.8900588) \quad x \quad (A - 27.5484329)] \}
\end{aligned}$$

Technology Group 5--Normal Emitters

$$V_i = \quad \{ [(0.002101) \quad x \quad (S - 163.0367287)] + \\
[(0.028814) \quad x \quad (A - 27.5484329)] \}$$

Technology Group 6--Normal Emitters

$$\begin{aligned}
V_i = \quad & \{ [(-0.001137) \quad x \quad (X - 1.415043)] + \\
& [(0.000026978) \quad x \quad (S - 163.0367287)] + \\
& [(0.031237) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.000906) \quad x \quad (T50 - 205.153526)] + \\
& [(0.003223) \quad x \quad (T90 - 310.8900588)] + \\
& [(-0.005252) \quad x \quad (A - 27.5484329)] + \\
& [(0.000144) \quad x \quad (O - 6.536288)] + \\
& [(-0.032122) \quad x \quad (X - 1.415043)^2] + \\
& [(0.056280) \quad x \quad (RVP - 8.8858423)^2] + \\
& [(-2.9338 \times 10^{-5}) \quad x \quad (T50 - 205.153526)^2] + \\
& [(0.000592) \quad x \quad (A - 27.5484329)^2] + \\
& [(-4.5417 \times 10^{-5}) \quad x \quad (S - 163.0367287) \quad x \quad (O - 6.536288)] + \\
& [(0.000134) \quad x \quad (T90 - 310.8900588) \quad x \quad (A - 27.5484329)] + \\
& [(-0.000102) \quad x \quad (T90 - 310.8900588) \quad x \quad (O - 6.536288)] \}
\end{aligned}$$

Technology Group 7--Normal Emitters

$$\begin{aligned}
V_i = \quad & \{ [(-0.019786) \quad x \quad (X - 1.415043)] + \\
& [(0.000188) \quad x \quad (S - 163.0367287)] + \\
& [(-0.002006) \quad x \quad (T50 - 205.153526)] + \\
& [(0.000518) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.006082) \quad x \quad (A - 27.5484329)] + \\
& [(-0.000908) \quad x \quad (O - 6.536288)] \}
\end{aligned}$$

Technology Group 9--Normal Emitters

$$\begin{aligned}
V_i = \quad & \{ [(-0.044593) \quad x \quad (X - 1.415043)] + \\
& [(0.000510) \quad x \quad (S - 163.0367287)] + \\
& [(0.011983) \quad x \quad (RVP - 8.8858423)] + \\
& [(-0.005613) \quad x \quad (T50 - 205.153526)] +
\end{aligned}$$

$$\begin{aligned} & [(-0.000479) \quad x \quad (T90 - 310.8900588)] + \\ & [(0.023213) \quad x \quad (A - 27.5484329)] \} \end{aligned}$$

Technology Group 1--High Emitters

$$\begin{aligned} V_i = & \{ [(-0.084805) \quad x \quad (X - 1.415043)] + \\ & [(-9.318 \times 10^{-6}) \quad x \quad (S - 163.0367287)] + \\ & [(-0.008319) \quad x \quad (RVP - 8.8858423)] + \\ & [(-0.011126) \quad x \quad (T50 - 205.153526)] + \\ & [(0.003267) \quad x \quad (T90 - 310.8900588)] + \\ & [(0.030016) \quad x \quad (A - 27.5484329)] + \\ & [(-0.060196) \quad x \quad (O - 6.536288)] + \\ & [(0.002267) \quad x \quad (X - 1.415043) x \quad (T50 - 205.153526)] + \\ & [(0.000706) \quad x \quad (T90 - 310.8900588) x \quad (A - 27.5484329)] \} \end{aligned}$$

Technology Group 2--High Emitters

$$\begin{aligned} V_i = & \{ [(-0.084805) \quad x \quad (X - 1.415043)] + \\ & [(-9.318 \times 10^{-6}) \quad x \quad (S - 163.0367287)] + \\ & [(-0.008319) \quad x \quad (RVP - 8.8858423)] + \\ & [(0.003267) \quad x \quad (T90 - 310.8900588)] + \\ & [(0.008465) \quad x \quad (A - 27.5484329)] + \\ & [(0.008005) \quad x \quad (O - 6.536288)] + \\ & [(0.002267) \quad x \quad (X - 1.415043) x \quad (T50 - 205.153526)] + \\ & [(0.000706) \quad x \quad (T90 - 310.8900588) x \quad (A - 27.5484329)] \} \end{aligned}$$

Technology Group 3--High Emitters

$$\begin{aligned} V_i = & \{ [(-0.084805) \quad x \quad (X - 1.415043)] + \\ & [(-9.318 \times 10^{-6}) \quad x \quad (S - 163.0367287)] + \\ & [(-0.008319) \quad x \quad (RVP - 8.8858423)] + \\ & [(0.003267) \quad x \quad (T90 - 310.8900588)] + \\ & [(0.008465) \quad x \quad (A - 27.5484329)] + \\ & [(0.128266) \quad x \quad (O - 6.536288)] + \\ & [(0.002267) \quad x \quad (X - 1.415043) x \quad (T50 - 205.153526)] + \\ & [(0.000706) \quad x \quad (T90 - 310.8900588) x \quad (A - 27.5484329)] \} \end{aligned}$$

Technology Group 4--High Emitters

$$\begin{aligned} V_i = & \{ [(-0.084805) \quad x \quad (X - 1.415043)] + \\ & [(-9.318 \times 10^{-6}) \quad x \quad (S - 163.0367287)] + \\ & [(-0.008319) \quad x \quad (RVP - 8.8858423)] + \\ & [(-0.005727) \quad x \quad (T50 - 205.153526)] + \\ & [(0.003267) \quad x \quad (T90 - 310.8900588)] + \\ & [(0.008465) \quad x \quad (A - 27.5484329)] + \\ & [(0.008005) \quad x \quad (O - 6.536288)] + \\ & [(0.002267) \quad x \quad (X - 1.415043) x \quad (T50 - 205.153526)] + \\ & [(0.000706) \quad x \quad (T90 - 310.8900588) x \quad (A - 27.5484329)] \} \end{aligned}$$

Technology Group 5--High Emitters

$$V_i = \{ [(-0.084805) \times (X - 1.415043)] + [(-9.318 \times 10^{-6}) \times (S - 163.0367287)] + [(0.320593) \times (RVP - 8.8858423)] + [(0.003267) \times (T90 - 310.8900588)] + [(0.008465) \times (A - 27.5484329)] + [(0.008005) \times (O - 6.536288)] + [(0.002267) \times (X - 1.415043) \times (T50 - 205.153526)] + [(0.000706) \times (T90 - 310.8900588) \times (A - 27.5484329)] \}$$

Technology Group 7--High Emitters

$$V_i = \{ [(-0.084805) \times (X - 1.415043)] + [(-9.318 \times 10^{-6}) \times (S - 163.0367287)] + [(-0.008319) \times (RVP - 8.8858423)] + [(0.003267) \times (T90 - 310.8900588)] + [(0.008465) \times (A - 27.5484329)] + [(0.008005) \times (O - 6.536288)] + [(0.002267) \times (X - 1.415043) \times (T50 - 205.153526)] + [(0.000706) \times (T90 - 310.8900588) \times (A - 27.5484329)] \}$$

where,

VOC = Non-methane, non-ethane emissions of volatile organic compounds in grams/mile

X = Oxygen content of the fuel in terms of weight percent

S = Sulfur content of the fuel in terms of parts per million by weight

O = Olefin content of the fuel in terms of volume percent

A = Aromatics content of the fuel in terms of volume percent

T90 = 90 percent distillation temperature of the fuel in terms of degrees Fahrenheit

T50 = 50 percent distillation temperature of the fuel in terms of degrees Fahrenheit

RVP = Reid vapor pressure of the fuel in terms of pounds per square inch

2. Exhaust NO_x Emissions

$$\text{Exhaust NO}_x \text{ (grams/mile)} = \sum k_i W_i e^{N_i}$$

VALUES OF k_i AND W_i FOR TECHNOLOGY GROUPS
WITHIN NORMAL AND HIGH EMITTERS - NO_x

TECHNOLOGY GROUP	NORMAL EMITTERS		HIGH EMITTERS	
	k_i	W_i	k_i	W_i
1	0.666296	0.219562	0.566758	0.043922
2	0.656289	0.239684	0.509666	0.047948
3	0.555082	0.182016	0.566758	0.036411
4	0.606598	0.100704	0.566758	0.020145
5	0.587796	0.036002	0.566758	0.007202
6	0.698742	0.000104	0	0
7	0.532033	0.043846	0.566758	0.008771
8	0	0	0	0
9	0.495686	0.013682	0	0

Technology Group 1--Normal Emitters

$$N_i = \{ [(0.02126866) \times (X - 1.415043)] + [(0.00095136) \times (S - 163.0367287)] + [(0.02738837) \times (RVP - 8.8858423)] + [(-0.00141286) \times (T50 - 205.153526)] + [(-0.0012709) \times (T90 - 310.8900588)] + [(0.0014277) \times (A - 27.5484329)] + [(0.0017607) \times (O - 6.536288)] + [(-2.930 \times 10^{-6}) \times (S - 163.0367287)^2] + [(-0.00932084) \times (RVP - 8.8858423)^2] + [(-0.00062386) \times (A - 27.5484329)^2] + [(0.00132136) \times (O - 6.536288)^2] + [(0.00012035) \times (X - 1.415043) \times (S - 163.0367287)] + [(0.02056244) \times (X - 1.415043) \times (RVP - 8.8858423)] + [(-0.0030604) \times (X - 1.415043) \times (A - 27.5484329)] + [(-0.0036465) \times (X - 1.415043) \times (O - 6.536288)] + [(-0.00017258) \times (S - 163.0367287) \times (RVP - 8.8858423)] + [(-2.840 \times 10^{-6}) \times (S - 163.0367287) \times (T90 - 310.8900588)] + [(0.00002431) \times (S - 163.0367287) \times (A - 27.5484329)] + [(-6.262 \times 10^{-5}) \times (S - 163.0367287) \times (O - 6.536288)] + [(0.01071723) \times (RVP - 8.8858423) \times (O - 6.536288)] + [(-0.00030275) \times (T50 - 205.153526) \times (A - 27.5484329)] + [(0.000142) \times (T90 - 310.8900588) \times (A - 27.5484329)] \}$$

Technology Group 2--Normal Emitters

$$N_i = \{ [(0.019932) \quad x \quad (X - 1.415043)] + \\ [(0.000581) \quad x \quad (S - 163.0367287)] + \\ [(-0.032528) \quad x \quad (RVP - 8.8858423)] + \\ [(-0.000987) \quad x \quad (T50 - 205.153526)] + \\ [(-3.2535 \times 10^{-5})x \quad (T90 - 310.8900588)] + \\ [(0.005044) \quad x \quad (A - 27.5484329)] + \\ [(0.002063) \quad x \quad (O - 6.536288)] + \\ [(-2.743 \times 10^{-6}) x \quad (S - 163.0367287)^2] + \\ [(-0.000449) \quad x \quad (A - 27.5484329)^2] + \\ [(0.001026) \quad x \quad (O - 6.536288)^2] + \\ [(-0.003187) \quad x \quad (X - 1.415043) x (A - 27.5484329)] + \\ [(-0.003612) \quad x \quad (X - 1.415043) x (O - 6.536288)] + \\ [(-6.2131 \times 10^{-5})x \quad (S - 163.0367287) x (O - 6.536288)] + \\ [(-0.001611) \quad x \quad (RVP - 8.8858423) x (T50 - 205.153526)] + \\ [(-0.000222) \quad x \quad (T50 - 205.153526) x (A - 27.5484329)] + \\ [(-0.000114) \quad x \quad (T50 - 205.153526) x (O - 6.536288)] + \\ [(0.000066377) \quad x \quad (T90 - 310.8900588) x (A - 27.5484329)] \}$$

Technology Group 3--Normal Emitters

$$N_i = \{ [(-0.012437) \quad x \quad (X - 1.415043)] + \\ [(0.000656) \quad x \quad (S - 163.0367287)] + \\ [(-0.004452) \quad x \quad (RVP - 8.8858423)] + \\ [(0.001625) \quad x \quad (T50 - 205.153526)] + \\ [(-0.001492) \quad x \quad (T90 - 310.8900588)] + \\ [(0.003718) \quad x \quad (A - 27.5484329)] + \\ [(-0.000373) \quad x \quad (O - 6.536288)] + \\ [(0.000022259) \quad x \quad (T90 - 310.8900588)^2] + \\ [(-0.031243) \quad x \quad (X - 1.415043) x (RVP - 8.8858423)] + \\ [(-0.001296) \quad x \quad (X - 1.415043) x (A - 27.5484329)] + \\ [(0.000058084) \quad x \quad (S - 163.0367287) x (O - 6.536288)] + \\ [(-4.6496 \times 10^{-5})x \quad (T90 - 310.8900588) x (A - 27.5484329)] \}$$

Technology Group 4--Normal Emitters

$$N_i = \{ [(-0.000255) \quad x \quad (X - 1.415043)] + \\ [(0.00002802) \quad x \quad (S - 163.0367287)] + \\ [(-0.012719) \quad x \quad (RVP - 8.8858423)] + \\ [(-0.000655) \quad x \quad (T50 - 205.153526)] + \\ [(0.000481) \quad x \quad (T90 - 310.8900588)] + \\ [(0.005907) \quad x \quad (A - 27.5484329)] + \\ [(-0.007716) \quad x \quad (O - 6.536288)] + \\ [(0.024196) \quad x \quad (X - 1.415043)^2] + \\ [(0.0005) \quad x \quad (O - 6.536288)^2] + \\ [(-0.039059) \quad x \quad (X - 1.415043) x (RVP - 8.8858423)] +$$

$$\begin{aligned}
& [(-6.954 \times 10^{-6}) \quad x \quad (S - 163.0367287) x (T50 - 205.153526)] + \\
& [(8.352 \times 10^{-6}) \quad x \quad (S - 163.0367287) x (T90 - 310.8900588)] + \\
& [(-0.005318) \quad x \quad (RVP - 8.8858423) x (T50 - 205.153526)] + \\
& [(0.015089) \quad x \quad (RVP - 8.8858423) x (A - 27.5484329)] + \\
& [(-0.026145) \quad x \quad (RVP - 8.8858423) x (O - 6.536288)] + \\
& [(0.000249) \quad x \quad (A - 27.5484329) x (O - 6.536288)] \}
\end{aligned}$$

Technology Group 5--Normal Emitters

$$\begin{aligned}
N_i = \{ & [(-0.002232) \quad x \quad (X - 1.415043)] + \\
& [(-0.000478) \quad x \quad (S - 163.0367287)] + \\
& [(-0.085175) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.001234) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.005006) \quad x \quad (A - 27.5484329)] + \\
& [(-0.00689) \quad x \quad (O - 6.536288)] + \\
& [(-0.007925) \quad x \quad (X - 1.415043) x (A - 27.5484329)] + \\
& [(-0.048043) \quad x \quad (RVP - 8.8858423) x (O - 6.536288)] + \\
& [(0.002331) \quad x \quad (T50 - 205.153526) x (O - 6.536288)] \}
\end{aligned}$$

Technology Group 6--Normal Emitters

$$\begin{aligned}
N_i = \{ & [(0.02366) \quad x \quad (X - 1.415043)] + \\
& [(-0.000113) \quad x \quad (S - 163.0367287)] + \\
& [(0.048056) \quad x \quad (RVP - 8.8858423)] + \\
& [(-0.000392) \quad x \quad (T50 - 205.153526)] + \\
& [(-0.001254) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.002309) \quad x \quad (A - 27.5484329)] + \\
& [(0.001333) \quad x \quad (O - 6.536288)] + \\
& [(-0.024869) \quad x \quad (X - 1.415043)^2] + \\
& [(8.700 \times 10^{-7}) \quad x \quad (S - 163.0367287)^2] + \\
& [(-0.00011) \quad x \quad (X - 1.415043) x (S - 163.0367287)] + \\
& [(0.038753) \quad x \quad (X - 1.415043) x (RVP - 8.8858423)] + \\
& [(-0.000281) \quad x \quad (X - 1.415043) x (T90 - 310.8900588)] + \\
& [(-0.00016) \quad x \quad (A - 27.5484329) x (O - 6.536288)] \}
\end{aligned}$$

Technology Group 7--Normal Emitters

$$\begin{aligned}
N_i = \{ & [(-0.027592) \quad x \quad (X - 1.415043)] + \\
& [(0.001117) \quad x \quad (S - 163.0367287)] + \\
& [(-0.065016) \quad x \quad (RVP - 8.8858423)] + \\
& [(-0.003424) \quad x \quad (T50 - 205.153526)] + \\
& [(0.006662) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.003223) \quad x \quad (A - 27.5484329)] + \\
& [(-0.001434) \quad x \quad (O - 6.536288)] + \\
& [(0.001863) \quad x \quad (S - 163.0367287) x (RVP - 8.8858423)] + \\
& [(-8.3073 \times 10^{-5}) x \quad (S - 163.0367287) x (A - 27.5484329)] \}
\end{aligned}$$

Technology Group 9--Normal Emitters

$$N_i = \{ [(-0.002506) \quad x \quad (X - 1.415043)] + \\ [(0.00038) \quad x \quad (S - 163.0367287)] + \\ [(-0.031737) \quad x \quad (RVP - 8.8858423)] + \\ [(0.003055) \quad x \quad (T90 - 310.8900588)] + \\ [(0.006416) \quad x \quad (O - 6.536288)] + \\ [(0.041083) \quad x \quad (X - 1.415043)^2] + \\ [(0.001527) \quad x \quad (T50 - 205.153526) x (O - 6.536288)] \}$$

Technology Group 1--High Emitters

$$N_i = \{ [(0.043634) \quad x \quad (X - 1.415043)] + \\ [(0.000354) \quad x \quad (S - 163.0367287)] + \\ [(0.016836) \quad x \quad (RVP - 8.8858423)] + \\ [(0.003464) \quad x \quad (T90 - 310.8900588)] + \\ [(0.017135) \quad x \quad (A - 27.5484329)] + \\ [(-0.007396) \quad x \quad (O - 6.536288)] + \\ [(-0.028373) \quad x \quad (X - 1.415043)^2] + \\ [(0.001747) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] \}$$

Technology Group 2--High Emitters

$$N_i = \{ [(0.043634) \quad x \quad (X - 1.415043)] + \\ [(0.000354) \quad x \quad (S - 163.0367287)] + \\ [(0.140496) \quad x \quad (RVP - 8.8858423)] + \\ [(0.010054) \quad x \quad (T50 - 205.153526)] + \\ [(0.003464) \quad x \quad (T90 - 310.8900588)] + \\ [(0.017135) \quad x \quad (A - 27.5484329)] + \\ [(-0.007396) \quad x \quad (O - 6.536288)] + \\ [(-0.028373) \quad x \quad (X - 1.415043)^2] + \\ [(0.001747) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] \}$$

Technology Group 3--High Emitters

$$N_i = \{ [(0.043634) \quad x \quad (X - 1.415043)] + \\ [(0.000354) \quad x \quad (S - 163.0367287)] + \\ [(0.016836) \quad x \quad (RVP - 8.8858423)] + \\ [(0.003464) \quad x \quad (T90 - 310.8900588)] + \\ [(0.017135) \quad x \quad (A - 27.5484329)] + \\ [(-0.007396) \quad x \quad (O - 6.536288)] + \\ [(-0.028373) \quad x \quad (X - 1.415043)^2] + \\ [(0.001747) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] \}$$

Technology Group 4--High Emitters

$$N_i = \{ [(0.043634) \quad x \quad (X - 1.415043)] + \\ [(0.000354) \quad x \quad (S - 163.0367287)] + \\ [(0.016836) \quad x \quad (RVP - 8.8858423)] + \\ [(0.003464) \quad x \quad (T90 - 310.8900588)] + \\ [(0.017135) \quad x \quad (A - 27.5484329)] + \\ [(-0.007396) \quad x \quad (O - 6.536288)] + \\ [(-0.028373) \quad x \quad (X - 1.415043)^2] + \\ [(0.001747) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] \}$$

Technology Group 5--High Emitters

$$N_i = \{ [(0.043634) \quad x \quad (X - 1.415043)] + \\ [(0.000354) \quad x \quad (S - 163.0367287)] + \\ [(0.016836) \quad x \quad (RVP - 8.8858423)] + \\ [(0.003464) \quad x \quad (T90 - 310.8900588)] + \\ [(0.017135) \quad x \quad (A - 27.5484329)] + \\ [(-0.007396) \quad x \quad (O - 6.536288)] + \\ [(-0.028373) \quad x \quad (X - 1.415043)^2] + \\ [(0.001747) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] \}$$

Technology Group 7--High Emitters

$$N_i = \{ [(0.043634) \quad x \quad (X - 1.415043)] + \\ [(0.000354) \quad x \quad (S - 163.0367287)] + \\ [(0.016836) \quad x \quad (RVP - 8.8858423)] + \\ [(0.003464) \quad x \quad (T90 - 310.8900588)] + \\ [(0.017135) \quad x \quad (A - 27.5484329)] + \\ [(-0.007396) \quad x \quad (O - 6.536288)] + \\ [(-0.028373) \quad x \quad (X - 1.415043)^2] + \\ [(0.001747) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] \}$$

where,

NO_x = NO_x emissions in grams/mile

X = Oxygen content of the fuel in terms of weight percent

S = Sulfur content of the fuel in terms of parts per million by weight

O = Olefin content of the fuel in terms of volume percent

A = Aromatics content of the fuel in terms of volume percent

T90 = 90 percent distillation temperature of the fuel in terms of degrees Fahrenheit

T50 = 50 percent distillation temperature of the fuel in terms of degrees Fahrenheit

RVP = Reid vapor pressure of the fuel in terms of pounds per square inch

EXHAUST TOXIC EQUATIONS

3. EXHAUST BENZENE EMISSIONS

EXHB = Exhaust Benzene (milligrams/mile) = $\sum k_i W_i e^{V_i}$

VALUES OF k_i AND W_i FOR TECHNOLOGY GROUPS (NORMAL EMITTERS ONLY)

TECHNOLOGY GROUP	NORMAL EMITTERS		HIGH EMITTERS	
	k_i (mg/mile)	W_i	k_i	W_i
1	21.45318	0.29587786	---	---
2	19.10029	0.32299140	---	---
3	21.77050	0.24528158	---	---
4	22.15558	0.13570703	---	---
5	0	0	---	---
6	25.27965	0.00014039	---	---
7	0	0	---	---
8	0	0	---	---
9	0	0	---	---

Technology Group 1--Normal Emitters

$$V_i = \{ [(0.015478) \times (X - 1.415043)] + [(0.002349) \times (S - 163.0367287)] + [(0.0383230) \times (RVP - 8.8858423)] + [(0.0035930) \times (T50 - 205.153526)] + [(0.000153) \times (T90 - 310.8900588)] + [(0.021524) \times (A - 27.5484329)] + [(0.014348) \times (O - 6.536288)] + [(0.3245210) \times (B - 1.6700)] + [(-0.08392) \times (X - 1.415043)^2] + [(-5.912 \times 10^{-6}) \times (S - 163.0367287)^2] +$$

$$\begin{aligned}
& [(0.000077018) \quad x \quad (T50 - 205.153526)^2] + \\
& [(0.063261) \quad x \quad (B - 1.670)^2] + \\
& [(0.001679) \quad x \quad (S - 163.0367287) x (RVP - 8.8858423)] + \\
& [(-0.00084) \quad x \quad (O - 6.536288) x (A - 27.5484329)] + \\
& [(-0.017926) \quad x \quad (B - 1.6700) x (A - 27.5484329)] \}
\end{aligned}$$

Technology Group 2--Normal Emitters

$$\begin{aligned}
V_i = \{ & [(0.019141) \quad x \quad (X - 1.415043)] + \\
& [(0.000314) \quad x \quad (S - 163.0367287)] + \\
& [(0.0502370) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.0022020) \quad x \quad (T50 - 205.153526)] + \\
& [(0.000182) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.019210) \quad x \quad (A - 27.5484329)] + \\
& [(0.007126) \quad x \quad (O - 6.536288)] + \\
& [(0.239875) \quad x \quad (B - 1.6700)] + \\
& [(-0.000455) \quad x \quad (S - 163.0367287) x (X - 1.415043)] + \\
& [(0.004277) \quad x \quad (X - 1.415043) x (A - 27.5484329)] + \\
& [(0.005281) \quad x \quad (O - 6.536288) x (X - 1.415043)] + \\
& [(-0.007571) \quad x \quad (RVP - 8.8858423) x (A - 27.5484329)] + \\
& [(0.000097) \quad x \quad (T50 - 205.153526) x (T90 - 310.8900588)] + \\
& [(0.000695) \quad x \quad (T50 - 205.153526) x (A - 27.5484329)] + \\
& [(-0.000317) \quad x \quad (T90 - 310.8900588) x (A - 27.5484329)] + \\
& [(-0.000461) \quad x \quad (A - 27.5484329) x (O - 6.536288)] \}
\end{aligned}$$

Technology Group 3--Normal Emitters

$$\begin{aligned}
V_i = \{ & [(0.041395) \quad x \quad (X - 1.415043)] + \\
& [(0.001409) \quad x \quad (S - 163.0367287)] + \\
& [(0.198910) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.004449) \quad x \quad (T50 - 205.153526)] + \\
& [(0.000444) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.031117) \quad x \quad (A - 27.5484329)] + \\
& [(-0.022166) \quad x \quad (O - 6.536288)] + \\
& [(0.288761) \quad x \quad (B - 1.6700)] + \\
& [(0.150214) \quad x \quad (RVP - 8.8858423)^2] + \\
& [(-8.313 \times 10^{-5}) \quad x \quad (S - 163.0367287) x (A - 27.5484329)] + \\
& [(-0.000745) \quad x \quad (S - 163.0367287) x (B - 1.6700)] + \\
& [(0.000332) \quad x \quad (O - 6.536288) x (T90 - 310.8900588)] + \\
& [(-0.060863) \quad x \quad (B - 1.6700) x (O - 6.536288)] \}
\end{aligned}$$

Technology Group 4--Normal Emitters

$$\begin{aligned}
V_i = \{ & [(-0.018827) \quad x \quad (X - 1.415043)] + \\
& [(0.000508) \quad x \quad (S - 163.0367287)] + \\
& [(-0.021681) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.002952) \quad x \quad (T50 - 205.153526)] + \\
& [(0.000056326) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.011072) \quad x \quad (A - 27.5484329)] +
\end{aligned}$$

$$\begin{aligned}
& [(-0.004795) \quad x \quad (O - 6.536288)] + \\
& [(0.475065) \quad x \quad (B - 1.6700)] + \\
& [(-0.079006) \quad x \quad (RVP - 8.8858423)^2] + \\
& [(0.001028) \quad x \quad (T50 - 205.153526) x (A - 27.5484329)] + \\
& [(-0.000357) \quad x \quad (T90 - 310.8900588) x (A - 27.5484329)] \}
\end{aligned}$$

Technology Group 6--Normal Emitters

$$\begin{aligned}
V_i = \{ & [(-0.02634) \quad x \quad (X - 1.415043)] + \\
& [(0.000090034) \quad x \quad (S - 163.0367287)] + \\
& [(0.101777) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.002629) \quad x \quad (T50 - 205.153526)] + \\
& [(-0.000481) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.023686) \quad x \quad (A - 27.5484329)] + \\
& [(-0.005395) \quad x \quad (O - 6.536288)] + \\
& [(0.205420) \quad x \quad (B - 1.6700)] + \\
& [(0.000136) \quad x \quad (T90 - 310.8900588)^2] + \\
& [(-0.098961) \quad x \quad (B - 1.6700) x (X - 1.415043)] + \\
& [(0.316539) \quad x \quad (B - 1.6700) x (RVP - 8.8858423)] \\
& [(-9.9 \times 10^{-5}) \quad x \quad (T50 - 205.153526) x (T90 - 310.8900588)] + \\
& [(0.000446) \quad x \quad (T50 - 205.153526) x (A - 27.5484329)] + \\
& [(-0.000648) \quad x \quad (A - 27.5484329) x (O - 6.536288)] \}
\end{aligned}$$

where,

EXHB = Exhaust Benzene emissions in mg/mile

X = Oxygen content of the fuel in terms of weight percent

S = Sulfur content of the fuel in terms of parts per million by weight

O = Olefin content of the fuel in terms of volume percent

A = Aromatics content of the fuel in terms of volume percent

T90 = 90 percent distillation temperature of the fuel in terms of degrees Fahrenheit

T50 = 50 percent distillation temperature of the fuel in terms of degrees Fahrenheit

RVP = Reid vapor pressure of the fuel in terms of pounds per square inch

B = Benzene content of the fuel in terms of volume percent

4. EXHAUST ACETALDEHYDE EMISSIONS

$$\text{ACET} = \text{Exhaust Acetaldehyde (milligrams/mile)} = \sum k_i W_i e^{v_i}$$

VALUES OF k_i AND W_i FOR TECHNOLOGY GROUPS (NORMAL EMITTERS ONLY)

TECHNOLOGY GROUP	NORMAL EMITTERS		HIGH EMITTERS	
	k_i (mg/mile)	W_i	k_i	W_i
1	1.538784	0.28218748	---	---
2	2.324295	0.30804812	---	---
3	1.619431	0.23393231	---	---
4	2.123347	0.12942782	---	---
5	0.615553	0.04627037	---	---
6	2.454408	0.00013390	---	---
7	0	0	---	---
8	0	0	---	---
9	0	0	---	---

Technology Group 1--Normal Emitters

$$V_i = \{ [(0.233948) \times (X - 1.415043)] + [(0.001334) \times (S - 163.0367287)] + [(0.124507) \times (RVP - 8.8858423)] + [(0.009635) \times (T50 - 205.153526)] + [(-0.001651) \times (T90 - 310.8900588)] + [(-0.015693) \times (A - 27.5484329)] + [(0.048612) \times (O - 6.536288)] + [(0.319761) \times (B - 1.6700)] + [(0.000175) \times (T50 - 205.153526)^2] + [(-0.002037) \times (O - 6.536288)^2] + [(0.217491) \times (X - 1.415043) \times (RVP - 8.8858423)] + [(0.228262) \times (B - 1.6700) \times (X - 1.415043)] + [(0.002988) \times (S - 163.0367287) \times (RVP - 8.8858423)] + [(0.000044128) \times (S - 163.0367287) \times (T50 - 205.153526)] + [(0.041565) \times (RVP - 8.8858423) \times (O - 6.536288)] + [(-0.001027) \times (O - 6.536288) \times (A - 27.5484329)] \}$$

Technology Group 2--Normal Emitters

$$V_i = \{ [(0.190472) \quad x \quad (X - 1.415043)] + \\ [(0.000133) \quad x \quad (S - 163.0367287)] + \\ [(0.147066) \quad x \quad (RVP - 8.8858423)] + \\ [(-0.00134) \quad x \quad (T50 - 205.153526)] + \\ [(-0.003495) \quad x \quad (T90 - 310.8900588)] + \\ [(-0.018295) \quad x \quad (A - 27.5484329)] + \\ [(0.023836) \quad x \quad (O - 6.536288)] + \\ [(0.224242) \quad x \quad (B - 1.6700)] + \\ [(0.171985) \quad x \quad (X - 1.415043)^2] + \\ [(-0.001579) \quad x \quad (O - 6.536288)^2] + \\ [(0.206415) \quad x \quad (B - 1.6700) \times (X - 1.415043)] + \\ [(0.000832) \quad x \quad (S - 163.0367287) \times (RVP - 8.8858423)] + \\ [(0.000063803) \quad x \quad (S - 163.0367287) \times (T50 - 205.153526)] + \\ [(0.000713) \quad x \quad (T50 - 205.153526) \times (O - 6.536288)] + \\ [(-0.013452) \quad x \quad (B - 1.6700) \times (T90 - 310.8900588)] \}$$

Technology Group 3--Normal Emitters

$$V_i = \{ [(0.381448) \quad x \quad (X - 1.415043)] + \\ [(0.001355) \quad x \quad (S - 163.0367287)] + \\ [(-0.019836) \quad x \quad (RVP - 8.8858423)] + \\ [(0.013919) \quad x \quad (T50 - 205.153526)] + \\ [(-0.002046) \quad x \quad (T90 - 310.8900588)] + \\ [(-0.012308) \quad x \quad (A - 27.5484329)] + \\ [(0.093610) \quad x \quad (O - 6.536288)] + \\ [(0.370079) \quad x \quad (B - 1.6700)] + \\ [(0.131749) \quad x \quad (X - 1.415043)^2] + \\ [(-0.00025) \quad x \quad (T50 - 205.153526)^2] + \\ [(-0.008143) \quad x \quad (O - 6.536288)^2] + \\ [(-0.011685) \quad x \quad (X - 1.415043) \times (A - 27.5484329)] + \\ [(-0.013095) \quad x \quad (X - 1.415043) \times (O - 6.536288)] + \\ [(0.306712) \quad x \quad (B - 1.6700) \times (X - 1.415043)] + \\ [(0.002199) \quad x \quad (S - 163.0367287) \times (RVP - 8.8858423)] + \\ [(0.000060864) \quad x \quad (S - 163.0367287) \times (T50 - 205.153526)] + \\ [(-0.00026) \quad x \quad (S - 163.0367287) \times (A - 27.5484329)] + \\ [(0.000354) \quad x \quad (T50 - 205.153526) \times (T90 - 310.8900588)] \}$$

Technology Group 4--Normal Emitters

$$V_i = \{ [(0.134764) \quad x \quad (X - 1.415043)] + \\ [(0.000089376) \quad x \quad (S - 163.0367287)] + \\ [(0.587319) \quad x \quad (RVP - 8.8858423)] + \\ [(0.005163) \quad x \quad (T50 - 205.153526)] + \\ [(0.002382) \quad x \quad (T90 - 310.8900588)] + \\ [(-0.017776) \quad x \quad (A - 27.5484329)] +$$

$$\begin{aligned} & [(0.060037) \quad \times (O - 6.536288)] + \\ & [(0.304886) \quad \times (B - 1.6700)] + \\ & [(-0.006057) \quad \times (O - 6.536288)^2] \} \end{aligned}$$

Technology Group 5--Normal Emitters

$$\begin{aligned} V_i = & \{ [(0.051249) \quad \times (T50 - 205.153526)] + \\ & [(0.685745) \quad \times (RVP - 8.8858423)^2] + \\ & [(0.029574) \quad \times (T50 - 205.153526) \times (X - 1.415043)] \} \end{aligned}$$

Technology Group 6--Normal Emitters

$$\begin{aligned} V_i = & \{ [(0.046425) \quad \times (X - 1.415043)] + \\ & [(-0.000526) \quad \times (S - 163.0367287)] + \\ & [(0.192235) \quad \times (RVP - 8.8858423)] + \\ & [(-0.002842) \quad \times (T50 - 205.153526)] + \\ & [(0.005043) \quad \times (T90 - 310.8900588)] + \\ & [(-0.006685) \quad \times (A - 27.5484329)] + \\ & [(0.018455) \quad \times (O - 6.536288)] + \\ & [(0.106039) \quad \times (B - 1.6700)] + \\ & [(0.190410) \quad \times (X - 1.415043)^2] + \\ & [(-0.000125) \quad \times (O - 6.536288) \times (S - 163.0367287)] + \\ & [(0.003509) \quad \times (RVP - 8.8858423) \times (T90 - 310.8900588)] \} \end{aligned}$$

where,

ACET = Exhaust acetaldehyde emissions in mg/mile

X = Oxygen content of the fuel in terms of weight percent

S = Sulfur content of the fuel in terms of parts per million by weight

O = Olefin content of the fuel in terms of volume percent

A = Aromatics content of the fuel in terms of volume percent

T90 = 90 percent distillation temperature of the fuel in terms of degrees Fahrenheit

T50 = 50 percent distillation temperature of the fuel in terms of degrees Fahrenheit

RVP = Reid vapor pressure of the fuel in terms of pounds per square inch

B = Benzene content of the fuel in terms of volume percent

5. EXHAUST FORMALDEHYDE EMISSIONS

$$\text{FORM} = \text{Exhaust Formaldehyde (milligrams/mile)} = \sum k_i W_i e^{F_i}$$

VALUES OF k_i AND W_i FOR TECHNOLOGY GROUPS WITHIN NORMAL EMITTERS

TECHNOLOG Y GROUP	NORMAL EMITTERS		HIGH EMITTERS	
	k_i	W_i	k_i	W_i
1	3.834308	0.282187479	---	---
2	6.067228	0.308048125	---	---
3	5.073907	0.233932306	---	---
4	1.601336	0.129427819	---	---
5	3.020367	0.046270372	---	---
6	4.994498	0.000133898	---	---
7	0	0	---	---
8	0	0	---	---
9	0	0	---	---

Technology Group 1--Normal Emitters

$$F_i = \{ [(0.070403) \quad x \quad (X - 1.415043)] + [(-0.000304) \quad x \quad (S - 163.0367287)] + [(0.02109) \quad x \quad (RVP - 8.8858423)] + [(0.013398) \quad x \quad (T50 - 205.153526)] + [(0.000863) \quad x \quad (T90 - 310.8900588)] + [(-0.00881) \quad x \quad (A - 27.5484329)] + [(0.012725) \quad x \quad (O - 6.536288)] + [(0.043598) \quad x \quad (B - 1.67)] + [(-0.000512) \quad x \quad (A - 27.5484329)^2] + [(0.013456) \quad x \quad (RVP - 8.8858423) \times (T50 - 205.153526)] + [(-0.001157) \quad x \quad (T50 - 205.153526) \times (O - 6.536288)] \}$$

Technology Group 2--Normal Emitters

$$F_i = \{ [(0.014476) \quad x \quad (X - 1.415043)] + [(-0.000659) \quad x \quad (S - 163.0367287)] + [(0.132107) \quad x \quad (RVP - 8.8858423)] + \}$$

$$\begin{aligned}
& [(0.002826) \quad \times \quad (T50 - 205.153526)] + \\
& [(0.003036) \quad \times \quad (T90 - 310.8900588)] + \\
& [(-0.012711) \quad \times \quad (A - 27.5484329)] + \\
& [(0.030848) \quad \times \quad (O - 6.536288)] + \\
& [(0.106899) \quad \times \quad (B - 1.67)] + \\
& [(-0.002308) \quad \times \quad (O - 6.536288)^2] + \\
& [(-0.097836) \quad \times \quad (X - 1.415043) \times (RVP - 8.8858423)] \}
\end{aligned}$$

Technology Group 3--Normal Emitters

$$\begin{aligned}
F_i = \{ & [(0.102778) \quad \times \quad (X - 1.415043)] + \\
& [(-0.000342) \quad \times \quad (S - 163.0367287)] + \\
& [(-0.181109) \quad \times \quad (RVP - 8.8858423)] + \\
& [(0.004512) \quad \times \quad (T50 - 205.153526)] + \\
& [(-0.001241) \quad \times \quad (T90 - 310.8900588)] + \\
& [(-0.011562) \quad \times \quad (A - 27.5484329)] + \\
& [(-0.055182) \quad \times \quad (O - 6.536288)] + \\
& [(0.164468) \quad \times \quad (B - 1.67)] + \\
& [(-0.002257) \quad \times \quad (A - 27.5484329)^2] + \\
& [(0.002626) \quad \times \quad (X - 1.415043) \times (T90 - 310.8900588)] + \\
& [(-0.006825) \quad \times \quad (X - 1.415043) \times (A - 27.5484329)] + \\
& [(0.000639) \quad \times \quad (T50 - 205.153526) \times (A - 27.5484329)] + \\
& [(0.000364) \quad \times \quad (T90 - 310.8900588) \times (O - 6.536288)] + \\
& [(0.001398) \quad \times \quad (A - 27.5484329) \times (O - 6.536288)] + \\
& [(-0.09106) \quad \times \quad (O - 6.536288) \times (B - 1.67)] \}
\end{aligned}$$

Technology Group 4--Normal Emitters

$$\begin{aligned}
F_i = \{ & [(0.065823) \quad \times \quad (X - 1.415043)] + \\
& [(-0.001507) \quad \times \quad (S - 163.0367287)] + \\
& [(-0.167831) \quad \times \quad (RVP - 8.8858423)] + \\
& [(-0.001537) \quad \times \quad (T50 - 205.153526)] + \\
& [(0.005703) \quad \times \quad (T90 - 310.8900588)] + \\
& [(0.006538) \quad \times \quad (A - 27.5484329)] + \\
& [(-0.005738) \quad \times \quad (O - 6.536288)] + \\
& [(0.256134) \quad \times \quad (B - 1.67)] + \\
& [(-0.228683) \quad \times \quad (RVP - 8.8858423)^2] + \\
& [(0.01732) \quad \times \quad (RVP - 8.8858423) \times (T50 - 205.153526)] + \\
& [(-0.044186) \quad \times \quad (O - 6.536288) \times (B - 1.67)] \}
\end{aligned}$$

Technology Group 5--Normal Emitters

$$\begin{aligned}
F_i = \{ & [(-0.031197) \quad \times \quad (T50 - 205.153526)] + \\
& [(-0.676188) \quad \times \quad (B - 1.67)] + \\
& [(0.001262) \quad \times \quad (X - 1.415043) \times (S - 163.0367287)] + \\
& [(-0.332229) \quad \times \quad (RVP - 8.8858423) \times (B - 1.67)] \}
\end{aligned}$$

Technology Group 6--Normal Emitters

$$F_i = \{ [(0.009547) \times (X - 1.415043)] + [(-0.0003275) \times (S - 163.0367287)] + [(-0.41979) \times (RVP - 8.8858423)] + [(0.008367) \times (T90 - 310.8900588)] + [(-0.004363) \times (A - 27.5484329)] + [(0.004008) \times (O - 6.536288)] + [(-0.033948) \times (B - 1.67)] + [(0.000010083) \times (S - 163.0367287)^2] + [(-0.262222) \times (RVP - 8.8858423)^2] + [(-0.244491) \times (X - 1.415043) \times (B - 1.67)] + [(0.005882) \times (RVP - 8.8858423) \times (T90 - 310.8900588)] + [(0.008091) \times (T90 - 310.8900588) \times (B - 1.67)] \}$$

where,

FORM = Exhaust formaldehyde emissions in mg/mile

X = Oxygen content of the fuel in terms of weight percent

S = Sulfur content of the fuel in terms of parts per million by weight

O = Olefin content of the fuel in terms of volume percent

A = Aromatics content of the fuel in terms of volume percent

T90 = 90 percent distillation temperature of the fuel in terms of degrees Fahrenheit

T50 = 50 percent distillation temperature of the fuel in terms of degrees Fahrenheit

RVP = Reid vapor pressure of the fuel in terms of pounds per square inch

B = Benzene content of the fuel in terms of volume percent

6. EXHAUST 1,3 BUTADIENE EMISSIONS

$$\text{BUTA} = \text{Exhaust 1,3 Butadiene (milligrams/mile)} = \sum k_i W_i e^{V_i}$$

VALUES OF k_i AND W_i FOR TECHNOLOGY GROUPS (NORMAL EMITTERS ONLY)

TECHNOLOGY GROUP	NORMAL EMITTERS		HIGH EMITTERS	
	k_i (mg/mile)	W_i	k_i	W_i
1	2.213974	0.29587786	---	---
2	3.269410	0.32299140	---	---
3	6.741066	0.24528158	---	---
4	3.159243	0.13570703	---	---
5	0	0	---	---
6	2.503301	0.00014039	---	---
7	0	0	---	---
8	0	0	---	---
9	0	0	---	---

Technology Group 1--Normal Emitters

$$V_i = \{ [(0.012945) \times (X - 1.415043)] + [(0.000643) \times (S - 163.0367287)] + [(0.067850) \times (RVP - 8.8858423)] + [(0.006647) \times (T50 - 205.153526)] + [(0.005098) \times (T90 - 310.8900588)] + [(-0.004155) \times (A - 27.5484329)] + [(0.053713) \times (O - 6.536288)] + [(0.082166) \times (B - 1.6700)] + [(-5.224 \times 10^{-6}) \times (S - 163.0367287)^2] + [(0.000129) \times (T50 - 205.153526)^2] + [(-0.000449) \times (A - 27.5484329)^2] + [(-0.00017) \times (S - 163.0367287) \times (O - 6.536288)] + [(0.004313) \times (T90 - 310.8900588) \times (RVP - 8.8858423)] \}$$

Technology Group 2--Normal Emitters

$$V_i = \{ [(0.005339) \times (X - 1.415043)] + [(-0.000105) \times (S - 163.0367287)] +$$

$$\begin{aligned}
& [(-0.075697) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.003831) \quad x \quad (T50 - 205.153526)] + \\
& [(0.003926) \quad x \quad (T90 - 310.8900588)] + \\
& [(-0.006371) \quad x \quad (A - 27.5484329)] + \\
& [(0.02016) \quad x \quad (O - 6.536288)] + \\
& [(0.077113) \quad x \quad (B - 1.6700)] + \\
& [(0.052837) \quad x \quad (RVP - 8.8858423) x (X - 1.415043)] + \\
& [(-0.003834) \quad x \quad (X - 1.415043) x (T50 - 205.153526)] + \\
& [(0.001324) \quad x \quad (T90 - 310.8900588) x (X - 1.415043)] + \\
& [(-0.022072) \quad x \quad (O - 6.536288) x (B - 1.6700)] \}
\end{aligned}$$

Technology Group 3--Normal Emitters

$$\begin{aligned}
V_i = \{ & [(0.177873) \quad x \quad (X - 1.415043)] + \\
& [(-0.001865) \quad x \quad (S - 163.0367287)] + \\
& [(-0.047321) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.011285) \quad x \quad (T50 - 205.153526)] + \\
& [(-0.010833) \quad x \quad (T90 - 310.8900588)] + \\
& [(-0.018904) \quad x \quad (A - 27.5484329)] + \\
& [(0.012441) \quad x \quad (O - 6.536288)] + \\
& [(0.535686) \quad x \quad (B - 1.6700)] + \\
& [(-0.001624) \quad x \quad (A - 27.5484329)^2] + \\
& [(-0.011535) \quad x \quad (X - 1.415043) x (A - 27.5484329)] + \\
& [(-0.002883) \quad x \quad (S - 163.0367287) x (RVP - 8.8858423)] + \\
& [(-0.000347) \quad x \quad (O - 6.536288) x (S - 163.0367287)] + \\
& [(0.009957) \quad x \quad (T90 - 310.8900588) x (RVP - 8.8858423)] + \\
& [(0.000609) \quad x \quad (T90 - 310.8900588) x (O - 6.536288)] + \\
& [(-0.018306) \quad x \quad (T90 - 310.8900588) x (B - 1.6700)] + \\
& [(0.001223) \quad x \quad (A - 27.5484329) x (O - 6.536288)] \}
\end{aligned}$$

Technology Group 4--Normal Emitters

$$\begin{aligned}
V_i = \{ & [(-0.009513) \quad x \quad (X - 1.415043)] + \\
& [(-0.000563) \quad x \quad (S - 163.0367287)] + \\
& [(-0.019244) \quad x \quad (RVP - 8.8858423)] + \\
& [(0.001092) \quad x \quad (T50 - 205.153526)] + \\
& [(0.004607) \quad x \quad (T90 - 310.8900588)] + \\
& [(0.000524) \quad x \quad (A - 27.5484329)] + \\
& [(0.013224) \quad x \quad (O - 6.536288)] + \\
& [(0.337679) \quad x \quad (B - 1.6700)] + \\
& [(0.000085623) \quad x \quad (T90 - 310.8900588)^2] + \\
& [(-0.004985) \quad x \quad (X - 1.415043) x (A - 27.5484329)] \}
\end{aligned}$$

Technology Group 6--Normal Emitters

$$\begin{aligned}
V_i = \{ & [(0.083176) \quad x \quad (X - 1.415043)] + \\
& [(-0.003067) \quad x \quad (S - 163.0367287)] + \\
& [(-0.45626) \quad x \quad (RVP - 8.8858423)] +
\end{aligned}$$

$$\begin{aligned}
& [(0.00562) \quad \times (T50 - 205.153526)] + \\
& [(0.005232) \quad \times (T90 - 310.8900588)] + \\
& [(-0.006116) \quad \times (A - 27.5484329)] + \\
& [(0.006062) \quad \times (O - 6.536288)] + \\
& [(-0.138741) \quad \times (B - 1.6700)] + \\
& [(0.000010491) \quad \times (S - 163.0367287)^2] + \\
& [(-0.287611) \quad \times (RVP - 8.8858423)^2] + \\
& [(0.005270) \quad \times (RVP - 8.8858423) \times (T90 - 310.8900588)] + \\
& [(0.013528) \quad \times (B - 1.6700) \times (T50 - 205.153526)] \}
\end{aligned}$$

where,

BUTA = Exhaust 1,3 butadiene emissions in mg/mile

X = Oxygen content of the fuel in terms of weight percent

S = Sulfur content of the fuel in terms of parts per million by weight

O = Olefin content of the fuel in terms of volume percent

A = Aromatics content of the fuel in terms of volume percent

T90 = 90 percent distillation temperature of the fuel in terms of degrees Fahrenheit

T50 = 50 percent distillation temperature of the fuel in terms of degrees Fahrenheit

RVP = Reid vapor pressure of the fuel in terms of pounds per square inch

B = Benzene content of the fuel in terms of volume percent

B. Complex Nonexhaust Emissions Model Equations

EPA proposes that nonexhaust emissions be modeled by the following relationships for Class 'B' areas:

$$\begin{aligned}
\text{VOC DI} &= [0.003318 \times (\text{RVP}^2)] - [0.03475 \times \text{RVP}] + 0.09960 \\
\text{VOC HS} &= [0.007018 \times (\text{RVP}^2)] - [0.07351 \times \text{RVP}] + 0.2107 \\
\text{VOC RL} &= [0.006630 \times (\text{RVP}^2)] - [0.03047 \times \text{RVP}] + 0.02377 \\
\text{VOC RF} &= [0.0009804 \times (\text{RVP}^2)] - [0.008922 \times \text{RVP}] + 0.05877
\end{aligned}$$

where

RVP = Reid vapor pressure of the fuel, in pounds per square inch

VOC DI = Diurnal nonmethane, nonethane VOC emissions, in grams per mile

VOC HS = Hot soak nonmethane, nonethane VOC emissions, in grams per mile

VOCRL = Running loss nonmethane, nonethane VOC emissions, in grams per mile
VOCRF = Refueling nonmethane, nonethane emissions, in grams per mile

Similarly, EPA proposes that nonexhaust emissions in Class 'C' areas be modeled by the following relationships:

$$\begin{aligned}\text{VOC DI} &= [0.003917 \times (\text{RVP}^2)] - [0.04828 \times \text{RVP}] + 0.1626 \\ \text{VOCHS} &= [0.008284 \times (\text{RVP}^2)] - [0.1021 \times \text{RVP}] + 0.3439 \\ \text{VOCRL} &= [0.003756 \times (\text{RVP}^2)] - [0.01780 \times \text{RVP}] + 0.06580 \\ \text{VOCRF} &= [0.0009804 \times (\text{RVP}^2)] - [0.008922 \times \text{RVP}] + 0.05877\end{aligned}$$

EPA proposes that nonexhaust benzene emissions be modeled in the same fashion as described in the simple model SNPRM. EPA proposes that benzene emissions be given by the following equations:

$$\begin{aligned}\text{RLBZ} &= [1000 \times (\text{BZV}\%/100) \times \text{RLVOC} \times (1.4448 - [0.0684 \times \text{OX}/2.0] - [0.080274 \times \text{RVP}])] \\ \text{REFBZ} &= [100 \times (\text{BZV}\%/100) \times \text{RFVOC} \times (1.3972 - [0.0591 \times \text{OX}/2.0] - [0.081507 \times \text{RVP}])] \\ \text{HSBZ} &= [1000 \times (\text{BZV}\%/100) \times \text{HSVOC} \times (1.4448 - [0.0684 \times \text{OX}/2.0] - [0.080274 \times \text{RVP}])] \\ \text{DIBZ} &= [1000 \times (\text{BZV}\%/100) \times \text{DVOC} \times (1.3758 - [0.0579 \times \text{OX}/2.0] - [0.080274 \times \text{RVP}])]\end{aligned}$$

where

RLBZ = Running loss benzene emissions, in milligrams per mile
REFBZ = Refueling benzene emissions, in milligrams per mile
HSBZ = Hot soak benzene emissions, in milligrams per mile
DIBZ = Diurnal benzene emissions, in milligrams per mile
BZV% = Volume percent benzene in the fuel
OX = Weight fraction of oxygen in the form of MTBE
RVP = Reid Vapor Pressure in pounds per square inch
VOCRL = Running loss VOC emissions in grams per mile
VOCRF = Refueling VOC emissions in grams per mile
VOCHS = Hot soak VOC emissions in grams per mile
VOC DI = Diurnal VOC emissions in grams per mile

The nonexhaust benzene equations are valid for oxygen levels in the form of MTBE up to 2.7 weight percent. Fuels with higher oxygen levels would be considered to have 2.7 weight percent oxygen content for the purposes of calculating nonexhaust benzene emissions.

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