
Fuel Effects on Exhaust Emissions from On-road Vehicles in MOVES2014

Final Report

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Final Report

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

NOTICE

This technical report does not necessarily represent final EPA decisions or positions. It is intended to present technical analysis of issues using data that are currently available. The purpose in the release of such reports is to facilitate the exchange of technical information and to inform the public of technical developments.

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1 Introduction

The MOVES2014 model estimates emissions inventories for different vehicle types operating on several fuels. Fuels in the model include gasoline, diesel, compressed natural gas (CNG), liquified petroleum gas, “ethanol (E-85)” and “electricity.” The “Ethanol” category includes blends of ethanol and gasoline in which the ethanol fraction exceeds 70 vol.%. Clearly, fully electrified vehicles do not emit exhaust pollutants, and will not be further discussed in this report. Note that MOVES2014 applies LPG only for the NONROAD component of the model. It is visible in the *fuelType* table and in the GUI due to sharing of tables between the on-road and NONROAD components of the model.

The different fuels are handled with widely varying levels of detail and sophistication, depending on factors such as the prevalence of use and availability of data. Given its historic and current importance in the market and in inventory modeling, the treatment for gasoline is the most extensive and detailed. At present, MOVES2014a is intended to estimate emissions from gasoline blends with ethanol up to 15 vol.%. The treatment for diesel and CNG is much simpler.

This document discusses adjustments or other calculations designed to account for changes in fuel properties on emissions of THC, CO, NO_x or PM. Similar calculations applied to emissions of air toxics are discussed in a separate report.¹

The draft version of this document underwent external peer review.² The comments of the two reviewers and the Agency’s responses are provided in Appendix B.

1.1 Gasoline

Estimation of emissions from gasoline plays a very important role in MOVES2014. Gasoline plays a substantial role in transportation, both in terms of the numbers of vehicles on U.S. roadways, and in terms of volumes consumed. Gasoline is also important in terms of historic and current policies and control measures, which often incorporate features involving control of fuel properties or content. Policies and programs that MOVES incorporates include reformulated gasoline (RFG), local fuel requirements, i.e., the so-called “boutique” gasolines, oxygenate blending requirements, and sulfur control requirements. Control of gasoline vapor pressure is also important, particularly for evaporative emissions, but is not discussed in this report, which is concerned with exhaust emissions. Estimation of evaporative hydrocarbons is discussed in a separate report.³

Oxygenate requirements reflected in the model include the use of methyl-tertiary-butyl-ether (MTBE) (as a historical factor) and ethanol mandates, including the renewable fuels standards (RFS1 and RFS2). The MOVES fuel supply currently reflects the fact that most gasolines in the U.S. contain approximately 10 vol.% ethanol. In addition, the fuel supply in MOVES2014 incorporates the introduction of gasolines containing up to 15 vol.% ethanol, i.e., “E15” fuels. The construction and composition of the default fuel supply is described in greater detail in a separate report.⁴

Sulfur requirements incorporated in the gasoline supply include the Tier-2 and Tier-3 emissions standards, which imposed reductions in the sulfur content of gasoline. Under the Tier-2 program, maximum and average sulfur levels were reduced from 300 to 80 and 120 to 30 ppm

from 2004 and 2006, respectively.⁵ Under the Tier-3 program, further reductions to an average level of 10 ppm will be realized by 2017.⁶

For gasoline fuels, the model applies “adjustments” to account for changes in selected fuel properties in the geographic area(s) and time periods covered in MOVES runs. The properties considered to be relevant include fuel-content parameters, as well as bulk properties. Fuel-content variables include levels of oxygenate, ethanol, olefins, aromatics and sulfur. Bulk properties include vapor pressure, distillation properties, expressed as temperatures (T50, T90) or as volumes evaporated at specific distillation temperatures (E200, E300).

The basis for calculating adjustments is the differences between “base” emissions, assumed to reflect the properties of a specific reference fuel, and “target” emissions, intended to reflect the set of “target” fuels in the areas and periods covered in a MOVES run. The concept and specific definitions of base gasolines are discussed below in Section 2.

During a run, MOVES combines emission rates and activity, e.g., vehicle-miles traveled, to generate the “base” emissions estimate, prior to applying adjustments for other factors, such as humidity, temperature and fuel properties. With respect to fuel properties, the “base estimate” is assumed to reflect the properties of an associated “base” gasoline. To indicate this aspect of model design, the emission rates stored in tables such as *emissionRate* or *emissionRateByAge* are designated as “mean base rates.”

Adjustments for sulfur are calculated separately and applied independently of those for other properties. For pre-2001 model year vehicles, the sulfur adjustments are calculated using an approach adapted from the MOBILE6 model, here designated as the “M6Sulf” model. The adaptation of this model for use in MOVES, incorporating “short-term” and “long-term” sulfur effects, is described Section 3.2. For 2001 and later model year vehicles, including those certified to Tier-2 standards, we have applied recent research to develop simple fractional adjustments for vehicles operating on gasolines with sulfur content < 30 ppm. The model, designated as the “T2LowSulf” model, is described in Section 3.3.

For other non-sulfur properties, approaches to calculating adjustments also differ for different subsets of vehicles.

For vehicles manufactured prior to MY 2001, we apply the “Complex Model” to calculate adjustments for CO and the “EPA Predictive Model” to calculate adjustments for THC and NO_x. The Complex and Predictive Models, described in Chapters 4 and 5, account for the effects of selected fuel properties, including oxygenates, aromatics, olefins, vapor pressure and distillation parameters. While broadly similar in their overall approaches, the data and analysis methods used in developing these models differ in important respects. The underlying datasets were composed of cycle aggregate emissions results, and thus we calculate and apply adjustments that are applied to both start and running exhaust emissions.

For vehicles applied after 2001, we apply a set of statistical models developed from the results of the “EPAct Phase-3 Project,” a large-scale controlled experiment conducted under a congressional mandate in the Energy Policy Act of 2005 (EPAct). Based on the results of this project, we apply adjustments for THC, CO, NO_x and PM_{2.5}, although in this case distinct adjustments are applied to start and running emissions. The design and analysis of these data incorporated advances in methods developed since development of the Complex and Predictive models. The development and application of these adjustments is described in Chapter 6.

Fuel sulfur plays yet another role in that MOVES2014 estimates emissions of sulfate (SO₄) as a component of the non-elemental-carbon component of PM_{2.5}. A refinement introduced in MOVES2014 is that this model also accounts for the contribution of lubricating oil to sulfate emissions.

The estimation of sulfate components is performed by the “sulfate calculator.” The calculator is designed so as to estimate sulfate emissions for user-specified fuels during model runs, by relating them to a set of “reference sulfate fractions” associated with “reference fuel sulfur levels.” The sulfate contribution from lubricating oil is assumed to be independent of the fuel sulfur level. The specific assumptions applied to gasoline fuels are described in Section 9.3.

In addition, MOVES2014 estimates emissions of sulfur dioxide (SO₂) as a function of gasoline consumption and sulfur level. Unlike the sulfate calculation, the SO₂ calculation assumes that all emissions are contributed by the fuel. As with the sulfate calculation, the SO₂ calculation uses the same structure for all fuels. Assumptions specific to gasoline are shown in Table 9-2 (page 114).

Lastly, fuels containing 70 to 85 vol.% ethanol (E85) have been available for many years and their use as transportation fuels has been growing. Vehicles designed to run on gasoline or such “high-level” ethanol blends are designated as flexible-fuel or “flex-fuel” vehicles (FFVs). MOVES2014 incorporates the capability of modeling emissions from FFVs running on fuels containing 70 to 85 vol.% ethanol. The algorithm for estimating the effects of E85 on emissions is described in Section 7.

2 “Base” and “Target” Gasolines

As previously described, the concept of “base” and “target” fuels is applied to gasoline fuels in the calculation of fuel adjustments using the Complex Model, EPA Predictive Model and the EPAct models. The bases and calculations of these adjustments are described in Chapters 4, 5, and 6, respectively.

Fuel adjustments are designed to represent differences between “base” and “target” emissions. “Base” emissions are emissions assumed to reflect a default set of conditions, including temperature, humidity and fuel properties. A “base gasoline” is defined as a set of selected gasoline properties assumed to be associated with, and implicit in, estimates of “base” emissions. A “base” emissions estimate is the result of a calculation in which base emission rates, i.e., from the *emissionRateByAge* table, are combined with appropriate measures of activity, i.e., vehicle miles traveled or numbers of vehicle starts, prior to the application of adjustments for temperature, fuel properties or other factors.

Several base gasolines are used in MOVES2014. Their properties are defined in the database table *BaseFuel*, and are further described in sub-section 2.1.

2.1 Base Gasolines

For gasolines, MOVES2014 uses two ‘base’ fuels for calculation of fuel adjustments for non-sulfur properties. These two fuels, designated as A and B, differ only in sulfur level. Fuel A is assigned a lower sulfur level applicable to vehicles in model year 2001 and later. Fuel B is assigned a higher sulfur level applicable to vehicles in model years 2000 and earlier. Fuels A and B are used in the calculation of fuel adjustments for HC, CO, NO_x and PM emissions.

In terms of properties other than sulfur, Base gasolines A and B are assumed to represent the “typical” gasoline in the Phoenix metropolitan area between calendar years 1995 and 2005. The emission rates for gaseous emissions from light-duty vehicles are based on random evaluation samples from the Phoenix Inspection and Maintenance Program during this time period. The development of these “I/M reference rates” (meanBaseRateIM) is described in detail in a separate report.⁷ Because fuel properties individual vehicles in the I/M lanes are unknown, we assume that the “averaged” fuel properties, based on fuel surveys in the same area during the same time period, can be associated with the average emission rates. The properties of each fuel are shown in Table 2-1 below.

2.2 Target Gasolines

The “target” gasoline is the gasoline which is to be evaluated for its effect on emissions, i.e., the fuel(s) assigned to the areas and periods covered in specific MOVES runs. The properties of target gasoline vary by county, year, and month. The MOVES2014 database contains a set of fuel formulations and associated fuel market share fractions for each county in the United States, for each month and for calendar years 1990 and 1999 through 2050. In addition to the default fuel formulations, the user may generate custom fuels through the “Fuel Wizard” feature. The development of the fuel supply tables and the “fuel wizard” is described in a separate document.⁴

Table 2-1. Properties of MOVES Base Gasolines.

Fuel Property Name	Fuel A	Fuel B
Fuel Sub-Type	Conventional	Conventional
fuelFormulationID	98	99
RVP (psi)	6.9	6.9
Sulfur Level (ppm)	30.0	90.0
Ethanol Volume (%)	0.0	0.0
MTBE Volume (%) ¹	0.0	0.0
ETBE Volume (%) ²	0.0	0.0
TAME Volume (%) ³	0.0	0.0
Aromatic Content (%)	26.1	26.1
Olefin Content (%)	5.6	5.6
Benzene Content (%)	1.0	1.0
E200 (%)	41.1	41.1
E300 (%)	83.1	83.1
T50 (°F)	218	218
T90 (°F)	329	329
Volume to percent Oxygen (%)	0.0	0.0
¹ Methyl tertiary-butyl ether, used as an oxygenate. ² Ethyl tertiary-butyl ether, used as an oxygenate. ³ Tertiary amyl-methyl ether, used as an oxygenate.		

2.2.1 Relevant Database Tables

The database tables listed below are relevant to the calculation of the fuel adjustments described in this report:

BaseFuel: this table contains properties for the base fuels used by MOVES2014 in calculation of fuel adjustments, as shown in Table 2-1 above.

FuelEngTechAssoc: This table stores associations of fuel type and engine technology that apply to each sourceType.

FuelModelName: This table identifies the individual statistical models used in applications of the Complex and EPA Predictive Models for CO and air toxics. The applications of these models in estimation of air-toxic emissions are discussed in a separate report.⁸

fuelModelWtFactor: Contains sets of factors used to weight the results of the various individual equations used in the application of the Complex Model. See Chapter 4.

FuelParameterName: This table defines the various fuel parameters included in MOVES calculations.

GeneralFuelRatio: This table is empty by design; it is populated during a model run.

GeneralFuelRatioExpression: this table contains mathematical expressions that calculate some of the fuel adjustments described in this chapter. It is described in greater detail in 6.5 (page 87).

The additional tables listed below are described in the fuel supply report:⁴

FuelFormulation,

FuelSupply,

RegionCounty,

FuelEngFraction,

FuelUsageFraction,

FuelWizardFactors,

E10FuelProperties.

3 Fuel Sulfur Effects

3.1 Introduction

Fuel sulfur content has long been understood to affect the performance of emission after-treatment catalysts in light-duty vehicles, where the sulfur and its oxides occupy active precious-metal sites and oxygen storage materials, reducing the catalyst's efficiency in removing pollutants. For light-duty vehicles, "three-way," or "oxidation-reduction" catalysts play a major role in reducing pollutant concentrations in exhaust streams. Catalysts contain precious metals and metal oxides to selectively oxidize hydrocarbons and carbon monoxide and reduce nitrogen oxides in the exhaust gases. Sulfur oxides from fuel combustion preferentially bind to active sites in the catalyst, inhibiting their ability to participate in the intended conversion reactions (a phenomenon often referred to as "sulfur poisoning"). The amount of sulfur retained by the catalyst is a function of the type and arrangement of active materials and coatings within the catalyst, its operating temperature, as well as the air-to-fuel ratio and concentration of sulfur in the exhaust gas.^{9,10}

Modern engines operate with rapid rich-lean oscillations that maintain the proper oxidation-reduction condition of the catalyst. Under typical driving conditions, however, a non-zero equilibrium level of sulfur is retained, which can accumulate over time. Regular operation at high temperatures under net reducing conditions can release much of the retained sulfur oxides from the catalyst, and can mitigate the effects of accumulated sulfur on catalyst efficiency. However, producing these conditions at sustained and/or regular intervals may accelerate thermal degradation of the catalyst and may also raise other challenges for emission control and fuel

economy. Additionally, failures to maintain high catalyst temperatures (e.g., due to cold weather, extended idle or rich operation), can severely impair the effectiveness of the catalyst in converting the products of combustion, leading to increases in emissions relative to a “clean” catalysts.

This chapter describes how MOVES2014 adjusts exhaust emissions of hydrocarbons (HC), carbon monoxide (CO), and nitrogen oxides (NO_x) in response to varying levels of fuel sulfur in gasoline. Because the quantity of sulfur present on the catalyst at any given time is primarily a function of operating temperature and the fuel sulfur level, the effects of gasoline sulfur content are modeled as though they are independent of the effects of other fuel properties.

Note that MOVES2014 assumes that there is no direct impact of fuel sulfur on criteria emissions from diesel vehicles. Note also that emissions of sulfate (SO₄) and sulfur dioxide (SO₂) are discussed in Chapter 9.

MOVES2014 includes two separate sulfur effects models. The two models are the “MOBILE6 Fuel Sulfur Model” (M6Sulf) and “Tier 2 Low Sulfur Model” (T2LowSulf). The M6Sulf model applies to (1) all model years for sulfur levels above 30 ppm, and (2) pre-2001 model years for sulfur level equal to and below 30 ppm. Section 3.2 details the M6Sulf model algorithm, as well as the underlying data and analyses, and discusses the minor changes and assumptions applied to adapt the M6Sulf model into the MOVES framework.

The T2LowSulf model applies only to 2001-and-later model year vehicles operating on sulfur levels equal to or below 30 ppm. Section 3.3 describes how the results of a study specifically designed to measure sulfur effects on Tier 2 gasoline vehicles were applied in MOVES2014. Previously, in MOVES2010, only the M6Sulf model was used to estimate the effects of fuel sulfur on emissions.

3.2 *The MOBILE6 Sulfur Model (M6Sulf)*

The M6Sulf model was developed through the analysis of several studies examining the effect of sulfur on exhaust emissions, described below. Vehicle technologies included in the analysis were Tier 0, Tier 1, Low-Emitting Vehicles (LEV), and Ultra Low-Emitting Vehicles (ULEV). For additional details, see “Fuel Sulfur Effects on Exhaust Emissions for MOBILE6.”¹¹

3.2.1 *Data Used in Developing the M6Sulf Model*

In developing the M6Sulf model, we relied on the following data sources:

Auto/Oil Phase I Sulfur Study¹²—As a part of the extensive testing program, ten 1989 model year light-duty gasoline vehicles (representing a subset of the fleet tested in all the other Auto/Oil studies) were tested using two fuels with sulfur levels of 466 and 49 ppm (other fuel parameters were held constant). The results indicated that overall HC, CO, and NO_x emissions were reduced by approximately 16%, 13% and 9%, respectively, when fuel sulfur content was reduced from the higher to the lower level.

Auto/Oil Phase II Sulfur Study¹³—This study expanded on the Phase I study by testing the same vehicle fleet over a wider range of sulfur levels with more intermediate points. This additional

work was performed to identify non-linear trends of emissions in relation to sulfur content. Two fuel sets were used. The first, termed “Part I”, was a five-fuel set ranging from a nominal sulfur level of 450 ppm down to 50 ppm in increments of 100 ppm. The second, termed “Part II”, was a three fuel set having sulfur levels of 50 ppm to 10 ppm in increments of 20 ppm. This study confirmed the results of the Phase I study and further found that reducing fuel sulfur from 50 ppm to 10 ppm resulted in a reduction in HC of 6% and CO of 10%; there was no statistically significant effect on NO_x emissions in this range.

T₅₀/T₉₀/Sulfur Study¹⁴—The study was designed to investigate possible non-linear impacts of the fuel distillation parameter T₉₀, interactive impacts of two fuel distillation parameters (T₅₀ and T₉₀) and sulfur on emissions from light-duty vehicles. Three vehicle fleets were tested: the Tier 0 vehicles assessed in the Phase I and Phase II Studies above (consisting of ten vehicles), a Federal Tier 1 fleet (consisting of six vehicles), and an “Advanced Technology” fleet (six production type LEV and ULEV vehicles). Only the Tier 0 and Tier 1 fleets were tested for their responses to changes in sulfur levels. Two fuel sets tested in this program were used to investigate the impact of fuel sulfur on exhaust emissions: a low T₉₀ set and a high T₉₀ set with approximate sulfur levels of 33 and 317 ppm.

API Extension Fuel Set¹⁵—In this program, the Tier 0 vehicle fleet (consisting of ten vehicles) from the Auto/Oil program was tested at sulfur levels of 450 and 900 ppm to investigate the impact of the higher levels of fuel sulfur observed in U.S. gasoline. The results from this program showed emission reductions of 5%, 2%, and 3% for HC, CO, and NO_x respectively, as a result of reducing sulfur from 900 to 450 ppm.

EPA RFG Phase I Study¹⁶—Phase I was an initial investigation of the impacts of oxygenates, volatility, distillation properties, and sulfur on emissions. The vehicles included in this program represented 1990 model-year or equivalent technology (Tier 0 vehicles). Two fuels examined in this program had differing sulfur levels (112 ppm and 371 ppm) with the other fuel parameters at approximately constant levels. The results indicated that decreasing sulfur from 371 ppm to 112 ppm caused a 5% reduction in HC emissions, a 7% reduction in NO_x emissions, and a 9% reduction in CO emissions in the tested fleet.

EPA RFG Phase II Study¹⁷—Phase II was a continuation of Phase I, investigating further the effects of oxygen content, oxygenate type, volatility, sulfur, olefins, and distillation parameters. Relevant testing included fuels with sulfur levels of 59 and 327 ppm. Again, vehicles with 1990 model-year or equivalent technology were tested. For the fleet tested, the results indicated that a reduction in sulfur from 327 to 59 ppm caused a 7% reduction in HC, a 5% reduction in NO_x emissions, and an 8% reduction in CO emissions.

API “Reversibility” Study¹⁸—American Petroleum Institute (API) tested a series of vehicles in response to the issue of sulfur reversibility in LEV and “advanced technology” vehicles. Sulfur “reversibility” refers to the ability of a vehicle to return to low emissions on low sulfur fuel after temporary use of high sulfur fuel. Only one of the vehicles was used in this analysis as part of the LEV emissions data set (all of which had approximately 100K mileage). The other vehicles from this test program were not included in the analysis either because: 1) they did not meet the criteria of mileage accumulation of 100K (see discussion below on why only the vehicles with the mileage accumulation of 100K was considered to be appropriate) or, 2) the testing was not completed at the time of the analysis.

CRC Sulfur/LEV Study¹⁹– This study involved six light-duty vehicles certified for sale in California as LEVs in 1997. Two fuel sets were investigated under this program: one fuel set was a California RFG with two sulfur levels (nominally 40 ppm and 150 ppm); the other set of five fuels had five different sulfur levels (nominally 40, 100, 150, 330, and 600 ppm). The vehicles were first tested in an “as-received” condition (average vehicle mileage of 10,000 miles) and with the catalysts bench-aged to simulate 100,000 miles of operation (although the oxygen sensors were original, low mileage sensors). The 10,000 mile emissions data will hereafter be referred to as the “10K data” and the 100,000 mile data will be referred to as the “100K data.” The conclusions from this study included:

- For the 10,000-mile catalysts, reducing sulfur from 600 to 40 ppm resulted in emission reductions of 46%, 63%, and 57% for NMHC, NO_x, and CO, respectively, over the FTP composite.
- For the aged 100,000-mile catalysts, reducing sulfur from 600 to 40 ppm resulted in emission reductions of 32%, 61%, and 46% for NMHC, NO_x, and CO, respectively, over the FTP composite.
- The fleet response to the changes in fuel sulfur level was found to be linear for the 10,000-mile catalysts and non-linear for the 100,000-mile catalysts. The effect of sulfur change was more pronounced at lower sulfur levels for the aged catalysts.

In the current analysis, only the 100K data was used since the other major LEV/ULEV testing program only tested vehicles with aged components to simulate 100,000 miles of driving. The emissions data from both fuel sets (conventional and RFG gasoline) were used in this analysis.

AAMA/AIAM Sulfur/LEV Study²⁰–This study tested 21 vehicles – 9 LEV LDVs, 1 LEV LDT1, 7 LEV LDT2s, and 4 ULEV LDVs. The vehicles were equipped with emission control components that were aged to mimic 100,000 miles of on-road driving. The base fuel used in the program was a California RFG with a nominal sulfur level of 40 ppm. The base fuel was then doped with sulfur compounds to obtain nominal sulfur levels of 100, 150, 330, and 600 ppm. Based on the 21 vehicle fleet, AAMA/AIAM reached the following conclusions:

- The emissions benefits of the technologies in low-emission vehicles are diminished as fuel sulfur level is increased above 40 ppm.
- The LEVs and ULEVs tested in this program showed a larger detrimental effect from fuel sulfur increases than the Tier 0 or Tier 1 vehicles tested in the Auto/Oil program.
- The emissions response of LEVs and ULEVs to fuel sulfur is non-linear for all pollutants and is more pronounced at lower sulfur levels.

3.2.2 Analysis of Short-Term Sulfur Effects

Unless otherwise specified, all data sets were analyzed using the following regression methodology. Individual fuel/vehicle data points were analyzed using a regression procedure in the SAS statistical software package “ABSORB”. The dummy variables were used to “absorb” the vehicles’ effect on emissions, thereby allowing the fuel sulfur effect to be isolated and better

approximated. This approach is similar to that used in the development of the reformulated gasoline Complex model in which a “dummy” variable was created for each vehicle in the data set. Repeat tests on vehicles (and for the same vehicle(s) used in different programs) at a given sulfur level were averaged to represent one data point. Emissions were regressed against the raw (“as-reported”) sulfur concentrations (ppm). In all cases, two different mathematical fits were considered in modeling the relationship between emissions and fuel sulfur level – log-log and log-linear. The selections were made based on the accuracy of the fit.

The original M6Sulf algorithm in MOBILE6 was based on the analyses that distinguished the vehicles into two emitter categories, “Normal” and “High”, based on the definition in Table 3-1 below.

Table 3-1. Definitions of “Normal” and “High” Emitter in the M6Sulf Model.

Emitter Category	Definition
Normal	Less than or equal to two times the emission standard for NO _x , or HC, or less than or equal to three times the emissions standard for CO
High	Greater than two times the emission standard for either NO _x , or HC, or greater than three times the emission standard for CO

The algorithm produced separate sulfur corrections for “Normal” and “High” emitters. Because MOVES2014 does not attempt to distinguish “normal” and “high” emitter classes and because the weights applied to effects for both classes were frequently about equal, the sets of model coefficients for “normal” and “high” emitters were regarded as independent models and assigned equal weights for consistency with the MOBILE6 model. For the purpose of describing the analyses that formed the basis of the M6Sulf model, the analyses of “Normal” and “High” emitters are presented separately in Section 3.2.2.1 and Section 3.2.2.1, respectively. Table 3-2 shows the numbers of vehicles in each emitter category for the studies included in developing the M6Sulf model.

Table 3-2. Number of Vehicles in Each of the Emitter Categories

Study	Normal Emitters	High Emitters
All Auto/Oil (all Tier 0 Vehicles)	10	0
EPA RFG Phase I (all Tier 0 Vehicles)	20	19
EPA RFG Phase II (all Tier 0 Vehicles)	24	15
Tier 1 T50/T90 Study (all Tier 1 vehicles)	6	0
CRC Sulfur/LEV Study (LEV and ULEV Vehicles)	12	0
AAMA/AIAM Sulfur/LEV Study (LEV and ULEV Vehicles and Trucks)	21	0
TOTALS:	93	34

3.2.2.1 Normal Emitters

3.2.2.1.1 Tier 0 Vehicles

The sulfur impacts for normal-emitting Tier 0 vehicles are based on combined analysis of the following studies: Auto/Oil data, the API extension fuel data, and the EPA RFG Phase I and Phase II data. Using the SAS “ABSORB” procedure described earlier, it was found that the log-log fit was consistently better than the log-linear fit. The resulting correlations are shown below in Table 3-3.

Table 3-3. Results of Regression Analysis for Tier 0 Normal-Emitting Vehicles

Pollutant	Emissions Process	Type of Regression Fit	Regression Coefficient	R ²
HC	Running	Ln-Ln	0.15262	0.947
CO	Running	Ln-Ln	0.19086	0.886
NO _x	Running	Ln-Ln	0.02083	0.944
HC	Start	Ln-Ln	0.0027436	0.959
CO	Start	Ln-Ln	-0.01792	0.860
NO _x	Start	Ln-Ln	0.04772	0.862

The estimated effects of the fuel sulfur level on emissions based on model predictions are shown in Table 3-4.

Table 3-4. Modeled Effects of Fuel Sulfur Level on Emissions for Tier 0 Normal-Emitting Vehicles

Pollutant	Emissions Process	% Increase in Emissions when Sulfur is Increased from 30 ppm to:			
		75 ppm	150 ppm	330 ppm	600 ppm
HC	Running	15.0	27.8	44.2	58.0
CO	Running	19.1	36.0	58.0	77.1
NO _x	Running	1.93	3.41	5.12	6.44
HC	Start	0.25	0.44	0.66	0.83
CO	Start	-1.63	-2.84	-4.21	-5.23
NO _x	Start	4.47	7.98	12.1	15.4

The Tier 0 analysis summarized in Table 3-3 and Table 3-4 applied to all normal emitters of Tier 0 and earlier vehicles (all vehicles equipped with a catalyst) since very little data is available to support an evaluation of the effect of sulfur on pre-Tier 0 vehicles. For vehicles not equipped with catalysts, sulfur is assumed to have no direct effect on exhaust emissions from those vehicles.

For comparison, Table 3-5 shows the estimated effects of reducing sulfur from 450 ppm to 50 ppm on emissions using the regressions listed in Table 3-3 for Tier 0 normal emitters and the effects computed from the Complex Model for normal emitters. The results are similar for CO, but the effects of sulfur on HC and NO_x estimated from M6Sulf model are smaller compared to the effects predicted by the Complex Model. This difference is probably due to the inclusion of the T₅₀/T₉₀ sulfur data set in the current analysis. Inspection of the T₅₀/T₉₀ sulfur data shows somewhat muted HC effects and much lower NO_x effects for sulfur variations. The T₅₀/T₉₀ sulfur data was not available at the time the Complex Model was constructed.

Table 3-5. Comparison of the Effects of Sulfur on Composite Emissions from M6Sulf Model and Complex Model when Sulfur is Reduced from 450 to 50 ppm

Model	HC (% Reduction)	NO _x (% Reduction)	CO (% Reduction)*
M6Sulf	13.0	6.6	15.4
Complex Model*	19.0	13.6	18.5

* CO emissions were not included in the original RFG Complex Model. The CO model estimates are based on the CO model developed separately (using the same statistical techniques used to construct the RFG Complex Model) from the RFG rulemaking and discussed in SAE paper 961214.²¹

3.2.2.1.2 Tier 1 Vehicles

For the analysis of Tier 1 vehicles, only one set of data, T50/T90 Sulfur, tested at the fuel sulfur levels of 330 ppm and 30 ppm was available. Because only two sulfur levels were available, the log-linear fit was chosen to represent the data. The regression coefficients and the estimated effects on emissions based on model predictions are shown in Table 3-6 and Table 3-7, respectively. It is interesting to note that the emission reductions from lower fuel sulfur are generally greater for Tier 1 vehicles than Tier 0 vehicles.

Table 3-6. Results of Regression Analysis for Tier 1 Normal-Emitting Vehicles

Pollutant	Emissions Process	Type of Regression Fit	Regression Coefficient	R ²
HC	Running	Ln-Linear	0.002457	0.818
CO	Running	Ln-Linear	0.001746	0.911
NO _x	Running	Ln-Linear	0.0006337	0.853
HC	Start	Ln-Linear	0.00009516	0.941
CO	Start	Ln-Linear	-0.0002338	0.820
NO _x	Start	Ln-Linear	0.0008023	0.692

Table 3-7. Modeled Effects of Fuel Sulfur Level on Emissions for Tier 1 Normal-Emitting Vehicles

Pollutant	Emissions Process	% Increase in Emissions when Sulfur is Increased from 30 ppm to:			
		75 ppm	150 ppm	330 ppm	600 ppm ¹
HC	Running	11.7	34.3	109.0	143.0
CO	Running	8.17	23.3	68.8	91.4
NO _x	Running	2.90	7.90	20.9	26.3
HC	Start	0.43	1.15	2.90	3.65
CO	Start	-1.05	-2.77	-6.77	-8.41
NO _x	Start	3.68	10.1	27.2	34.6

¹Please see the explanation below about how the effects at 600 ppm were estimated.

Since the underlying data for Tier 1 vehicles included the sulfur level of only up to 330 ppm, it would be inappropriate to extrapolate using the log-linear regression beyond 330 ppm.

Therefore, for any sulfur level between 330 ppm and 600 ppm (the high end of the sulfur range in MOVES), the following equations were used to estimate the effect of fuel sulfur on Tier 1 vehicles. The fractional effect for Tier-1 vehicles at any sulfur level $X > 330$ ppm ($f_{T1,X}$) is given by Equation 3-1,

$$f_{T1,X} = f_{T1,330} \left(\frac{f_{T0,X}}{f_{T0,330}} \right) \quad \text{Equation 3-1}$$

where:

$f_{T1,330}$ = the fractional change in emissions for Tier 1 vehicles at 330 ppm relative to a 30-ppm baseline (available in Table 3-7),

$f_{T0,X}$ = the fractional change in emissions for Tier 0 vehicles at level X relative to a 30-ppm baseline (can be estimated from Table 3-4),

$f_{T0,330}$ = the fractional change in emissions for Tier 0 vehicles at 330 ppm relative to a 30-ppm baseline (available in Table 3-4).

For example, using the equation above, the effect of increasing sulfur to 600 ppm from 30 ppm on running HC emissions for Tier 1 vehicles would be: $1.09 (0.58/0.442) = 1.43$ (i.e., 143%). The values 58.0% and 44.2% were obtained from Table 3-4 and 109.0% was obtained from Table 3-7.

3.2.2.1.3 LEVs and ULEVs

As discussed in Section 3.2.1 above, AAMA/AIAM and CRC Sulfur programs were used to estimate the effect of fuel sulfur on LEVs and ULEVs. While the analyses for Tier 0 and Tier 1 vehicles were based only on light-duty vehicles, the data for LEVs and ULEVs also included light-duty trucks. Separate analyses were conducted for light-duty vehicles (passenger cars and light trucks) and for light-duty trucks (LDT2, LDT3, and LDT4). These data were analyzed in the same manner as described above using the SAS “ABSORB” procedure.

Because we were unable to get the bag data from the testing programs to determine the start and running coefficients separately, the regression was run on the composite and the resulting coefficients were applied to both running and start emissions. Consistent with the findings from the AAMA/AIAM and CRC reports, log-log regression model was found to be a better fit for the data.

The regression coefficients for estimating the effects of fuel sulfur on emissions from LEV (and cleaner technology) are summarized in Table 3-8. Compared to Tier 0 and Tier 1 vehicles, ULEV and LEV vehicles were more sensitive to the changes in fuel sulfur levels.

Table 3-8. Results of Regression Analysis for normal-emitting LEVs and ULEVs.

Pollutant	Passenger cars (LDV)			Light Trucks (LDT2,3,4)		
	Composite Emissions	Running Emissions	Start Emissions	Composite Emissions	Running Emissions	Start Emissions
HC	0.168	0.168	0.168	0.125	0.125	0.125
CO	0.236	0.236	0.236	0.151	0.151	0.151
NO _x	0.351	0.351	0.351	0.146	0.146	0.146

3.2.2.1 High Emitters

The vehicles meeting the emissions criteria for high emitters (Table 3-1) were available only in the EPA RFG Phase 1 and 2 datasets (Table 3-2). These data were used to estimate regression coefficients for high-emitting Tier 0 vehicles, which were, however, also applied for LEV and Tier-2 vehicles. A log-linear fit was used since the volume of high-emitter data available was small and only two sulfur levels were tested in the EPA RFG programs. The regression coefficients for high emitters are shown in Table 3-9 and the corresponding emission effects are shown in Table 3-10.

Table 3-9. Results of Regression Analysis for Tier 0 High-Emitting Vehicles (Also applied for LEV and Tier-2 “High-Emitting” Vehicles.

Pollutant	Emissions Process	Type of Regression Fit	Regression Coefficient	R ²
HC	Running	Ln-Linear	1.138E-4	0.996
CO	Running	Ln-Linear	1.111E-4	0.993
NO _x	Running	Ln-Linear	2.848E-4	0.998
HC	Start	Ln-Linear	-2.227E-4	0.985
CO	Start	Ln-Linear	-5.336E-4	0.962
NO _x	Start	Ln-Linear	2.519E-4	0.889

Table 3-10. Effects of Fuel Sulfur Level on Emissions for Tier 0 High-Emitting Vehicles.

Pollutant	Emissions Process	% Increase in Emissions when Sulfur is Increased from 30 ppm to:			
		75 ppm	150 ppm	330 ppm	600 ppm
HC	Running	0.51	1.37	3.47	6.70
CO	Running	0.50	1.34	3.39	6.54
NO _x	Running	1.29	3.48	8.92	17.6
HC	Start	-1.00	-2.64	-6.46	-11.9
CO	Start	-2.37	-6.20	-14.8	-26.2
NO _x	Start	1.14	3.07	7.85	15.4

Table 3-11 compares the estimated effects of reducing sulfur from 450 ppm to 50 ppm on emissions using the regression coefficients listed in Table 3-9 for Tier 0 high emitters and the effects computed from the Complex Model for high emitters.

Table 3-11. Comparison of the Effects of Sulfur on Composite Emissions from Tier 0 High Emitters using M6Sulf Model and Complex Model when Sulfur is Reduced from 450 to 50 ppm.

Model	HC (% Reduction)	CO (% Reduction)*	NO _x (% Reduction)
M6Sulf	1.5	0.3	11.2
Complex Model ¹	-5.0	1.4	10.0

¹CO emissions were not in the original RFG Complex Model. The CO model developed separately (using the same statistical techniques used to construct the RFG Complex Model) and is discussed in SAE paper 961214¹³.

3.2.3 Analysis of Long-Term Sulfur Effects

In addition to adsorbing onto the surface of the catalyst and acting as a “poison,” sulfur can also penetrate into the precious metal layer, especially into palladium (the metal of choice for LEV catalysts), and into the oxygen storage material and further damage the catalyst. Full penetration may not have occurred during the very few miles of operation prior to short-term emission testing on high sulfur fuel. The short-term exposure in the test programs (evaluated previously in Section 3.2.2) typically consisted only of running several emission tests (FTP or LA4). Since each FTP is approximately 18 miles in length, the short-term exposure usually amounted to just under 100 miles of operation, all of which was in a controlled laboratory environment.

To address this concern, API and EPA conducted test programs on a total of six light-duty vehicles for sulfur sensitivity after both short-term and long-term exposures to sulfur.¹⁸ The long-term exposure consisted of between 1,500 and 4,000 miles of in-use operation over urban, rural, and highway roads. Two of the vehicles were 1999 models, while the other four were all 1998 models. All six were either LEV or ULEV vehicles. Three of the vehicles were equipped with catalyst systems aged to either 50,000 or 100,000 miles. The other three vehicles had low mileage catalyst systems aged to only about 4,000 miles.

All of the vehicles were tested for short-term exposure prior to the long-term testing. Each vehicle was tested using a FTP baseline tested on low sulfur fuel (30 or 40 ppm). The number of tests used to establish the baseline varied from two to four. The vehicles were then tested with the high sulfur fuel (EPA at 350 ppm, API at 540 ppm). Sulfur sensitivity was determined by calculating the percent increase in average emissions with the high sulfur fuel compared to the average emissions with the low sulfur fuel. Table 3-12 lists both the short-term and the long-term sulfur sensitivity data for all six vehicles.

In order to quantify the difference between short-term and long-term exposures, a fleet average emission rate was determined for both low and high sulfur fuels for each pollutant, for both long-term and short-term exposures. The percent change in emissions between low and high sulfur fuels was calculated, and the ratio of long-term sensitivity to the short-term sensitivity was then determined. As shown in Table 3-13, the percent increases from short-term to long-term were quite large, especially for hydrocarbon emissions. Statistical tests performed to assess the significance of the observed increases in sulfur sensitivity are discussed in Appendix B of the Tier 2 Regulatory Impact Analysis.²²

Table 3-12. Vehicle-by-Vehicle Short-Term vs. Long-Term Sulfur Sensitivity.

Vehicle	Sulfur Aging	Sulfur Level	Exhaust Tailpipe Emissions (g/mi)			Sulfur Sensitivity (%)		
			HC	CO	NOx	HC	CO	NOx
Accord	Short	30	0.031	0.351	0.092	12.0	36.3	69.4
		350	0.035	0.478	0.155			
	Long	30	0.033	0.330	0.09	21.7	121.1	158.5
		350	0.040	0.731	0.234			
Cavalier	Short	30	0.070	1.778	0.068	49.3	127.7	347.0
		350	0.105	4.048	0.303			
	Long	30	0.070	1.778	0.068	216.0	306.4	411.8
		350	0.223	7.224	0.324			
Altima	Short	40	0.041	0.788	0.061	43.9	34.3	83.6
		540	0.059	1.058	0.112			
	Long	40	0.041	0.788	0.061	39.0	25.3	116.4
		540	0.057	0.987	0.132			
Taurus	Short	40	0.033	0.522	0.075	54.5	59.4	34.7
		540	0.051	0.832	0.101			
	Long	40	0.033	0.522	0.075	121.2	151.0	56.0
		540	0.073	1.310	0.117			
Accord	Short	40	0.029	0.285	0.100	10.3	4.9	92.0
		540	0.032	0.299	0.192			
	Long	40	0.029	0.285	0.100	41.4	63.2	145.0
		540	0.041	0.465	0.245			
Avalon	Short	40	0.040	0.406	0.068	52.5	33.3	70.6
		540	0.061	0.541	0.116			
	Long	40	0.040	0.406	0.068	50.0	80.8	108.8
		540	0.060	0.734	0.142			

Table 3-13. Differences between Short-Term and Long-Term Sulfur Sensitivities

Average	Sulfur Sensitivity (%)			Ratio of long-term to short-term sensitivity		
	HC	CO	NOx	HC	CO	NOx
Short-Term	40.2	75.7	111.3	2.50	2.36	1.47
Long-Term	100.3	178.7	163.4			

3.2.4 Application in MOVES

In MOVES2014, the M6Sulf model is applied to (1) all model years for sulfur levels above 30 ppm, and (2) pre-2001 model years for sulfur levels equal to and below 30 ppm. In addition, the M6Sulf model is applied to all sourcetypes.

The M6Sulf model data, based on the analyses in Section 3.2.2, are stored in “*sulfurmodelcoeff*” table, described in Table 3-14.

Table 3-14. Description of the Database Table “sulfurmodelcoeff”

Field	Description	Values
processID	Identifies the emissions process.	1 = running exhaust 2 = start exhaust
pollutantID	Identifies the pollutant	1 = total hydrocarbons (THC) 2 = carbon monoxide (CO) 3 = nitrogen oxides (NO _x)
M6emitterID	Identifies the emitter classes. See “ <i>sulfurmodelname</i> ” table	1 = normal emitter 2 = high emitter ¹
sourcetypeID	Identifies vehicles by functional type.	11= motorcycle 21= passenger car 31=passenger truck 32=light commercial truck, etc.
fuelMYGroupID	The range of model year groups to which the sulfur coefficients are applied	e.g., 1960-1974, 1997-2000, etc.
sulfurFunctionID	Identifies the type of regression the coefficients are based on. See “ <i>sulfurmodelname</i> ” table	1 = log-log 2 = log-linear
sulfurCoeff	The sulfur coefficients from the regression analyses	See Section 3.2.2
¹ MOVES does not distinguish “high emitters” as such, but the calculator does apply both models and weights the results equally.		

3.2.4.1 Short-Term Sulfur Effects

The Short-Term Sulfur Effect estimates the short-term effects on emissions due to adsorption of sulfur onto the catalyst surface by calculating an adjustment to the base emissions as a function of the sulfur content of the gasoline. The initial calculations use Equation 3-2 and Equation 3-3 in cases where the log-log relationship is required (sulfurFunctionID = 1), or **Equation 3-4** and **Equation 3-5** when the log-linear relationship is required (sulfurFunctionID = 2).

In these equations, the coefficient (β) represents the *sulfurCoeff* field in the *sulfurModelCoeff* table, values of which are presented in 3.2.2 above. As shown in the tables, the *sulfurCoeff* varies by pollutant, process and “emitter status.”

The intermediate variable “sulfShortTarget” ($C_{\text{short,target}}$) is the correction factor for the sulfur level of the fuel being modeled, for which the sulfur content (x_s) is expressed in ppm. The parameter, $C_{\text{short,basis}}$, is the correction factor for the base sulfur (*sulfurBasis* variable in the *SulfurBase* table) level. The sulfur basis ($x_{S,\text{basis}}$) is always set at 30 ppm.

$$C_{\text{short,target}} = \exp(\beta \ln x_s) \quad \text{Equation 3-2}$$

$$C_{\text{short,basis}} = \exp(\beta \ln x_{S,\text{basis}}) \quad \text{Equation 3-3}$$

$$C_{\text{short,target}} = \exp(\beta x_s) \quad \text{Equation 3-4}$$

$$C_{\text{short,basis}} = \exp(\beta x_{S,\text{basis}}) \quad \text{Equation 3-5}$$

The Short-term sulfur effect (SulfAdj, $A_{S,\text{short}}$) for all groups is computed using Equation 3-6.

$$A_{S,short} = \frac{C_{short,target} - C_{short,basis}}{C_{short,basis}} \quad \text{Equation 3-6}$$

In this application of **Equation 3-6** the numerator is multiplied by 0.60 only for NO_x to represent high emitters, based on the analysis of the Complex Model which indicated that the NO_x sensitivity of high emitters is approximately 60 percent of the sensitivity for normal emitters.

3.2.4.2 Long-Term Sulfur Effects

As described in Section 3.2.3, the Long-Term Sulfur Effects are intended to account for reversible effects of prolonged exposure to sulfur in the catalyst. The values used in MOVES2014 (Table 3-13) are stored in the sulfurLongCoeff variable ($A_{S,long}$) in “*M6SulfurCoeff*” table. The values for sulfurLongCoeff are a function of pollutant. The long-term sulfur effects apply to LEV and cleaner vehicles and trucks. Tier 0 and Tier 1 vehicles and trucks only have the short-term sulfur effects. In addition, the sulfur levels of 30 ppm or less are assumed to have no long-term sulfur effects.

The short-term sulfur effects from Section 3.2.4.1 and multiplied by the long-term sulfur effects to produce the variable sulfAdj2 (A_2), as shown in Equation 3-7.

$$A_2 = A_{s,short} \times A_{s,long} \quad \text{Equation 3-7}$$

3.2.4.3 Sulfur Irreversibility Effects

In this step, the permanent effects of sulfur on emissions are computed. These effects are intended to represent the long-term emission impact of past exposure to high sulfur fuels, even when current fuels have lower sulfur levels. The irreversibility effects apply to only “LEV” and later (2001+ model year vehicles), and apply only to target fuel sulfur levels greater than 30 ppm sulfur. For model years 2003 and earlier and for fuel sulfur levels ≤ 30 ppm, the model does not calculate permanent effects. The same effects are applied to all three pollutants (HC, CO and NO_x) and processes (start and running).

If the fuel sulfur level is greater than 30 ppm but less than a specified “*maxIRFactorSulfur*” ($x_{S,cap}$), also stored in *M6SulfurCoeff*, Equation 3-8 is used to compute the “irreversible sulfur effect” ($A_{S,Irr}$, SulfIRR). The effect is applied as a function of model year group.

The *maxIRFactorSulfur* is applied as a function of model year group, as follows:

Model Year Group	Maximum S level
2001 – 2003	1,000 ppm
2004 – 2005	303 ppm
2006 – 2007	87 ppm
2008 +	80 ppm

$$A_{S,Irr} = \exp(\phi \ln x_{S,cap}) \quad \text{Equation 3-8}$$

If the selected sulfur level is greater than the maximum sulfur level, rather than using the value of the “cap” as the sulfur level, the actual sulfur level (x_S) is input to the **Equation 3-8** to calculate the irreversibility effect. However, sulfur levels above the maximum are not expected in normal use of the MOVES model.

3.2.4.4 Combining Short-Term, Long-Term and Irreversibility Sulfur Effects

Equation 3-9 combines all the sulfur effects described into a final sulfur effect, designated as $A_{S,3}$ or “sulfAdj3.” The effect is calculated as a multiplicative adjustment, and includes the short-term effects applied to the fuel basis ($C_{short,basis}$) from **Equation 3-3** or Equation 3-5, the combined short-term and long-term adjustment (A_2 , Equation 3-7) and the irreversibility effect $A_{S,Irr}$ (**Equation 3-8**). The two main terms in the expression are weighted by the factor w_{IR} (irreversibility factor), which takes a value of 0.425.²³

$$A_{S,3} = 1.0 + \left[w_{IR} \left(\frac{A_{S,Irr} - C_{short,basis}}{C_{short,basis}} \right) + (1.0 - w_{IR}) A_2 \right] \quad \text{Equation 3-9}$$

3.2.4.5 Sulfur Effects in Geographical Phase-In Areas (GPA)

During calendar years 2004-2006, the gasoline sulfur levels in the Sulfur “Geographical Phase-In Area” (Sulfur GPA) were allowed to remain higher than elsewhere in the nation. MOVES accounts for this difference with the calculation of “Sulfur GPA Effects.” The algorithm applies a maximum sulfur level of 330 ppm within designated “GPA areas,” most of which are located in the Rocky Mountains and are identified in the database table “*county*,” using the field “GPAFract.”

The sulfur adjustments in GPA are calculated using the same process as for other areas, except that the variable for the sulfur basis is assigned a different value. A value of 330 ppm, representing a typical worst case in a GPA scenario ($x_{S,GPAmax}$), is assigned in Equation 3-10 in place of the actual sulfur level in the fuel to be evaluated. The result $C_{short,GPA}$ is applied in Equation 3-11 with $C_{short,basis}$ to give the adjustment $A_{S,short,GPA}$, as shown below:

$$C_{short,GPA} = \exp \left(\beta \ln x_{S,GPAmax} \right) \quad \text{Equation 3-10}$$

$$A_{S,short,GPA} = \frac{C_{short,GPA} - C_{short,basis}}{C_{short,basis}} \quad \text{Equation 3-11}$$

As with non-GPA areas, the combined short- and long-term effect is calculated by multiplying the GPA short-term effect and the same long-term coefficient as used outside GPA areas, using Equation 3-12.

$$A_{2,GPA} = A_{S,short,GPA} \times A_{long} \quad \text{Equation 3-12}$$

Then, the equivalent of the adjustment $A_{S,3}$ for the GPA area ($A_{3,GPA}$) is calculated by applying Equation 3-13 as shown below.

$$A_{3,GPA} = 1.0 + \left(w_{IR} A_{2,GPA} + (1.0 - w_{IR}) A_2 \right) \quad \text{Equation 3-13}$$

For calendar years other than 2004, 2005, and 2006, or in areas where sulfur < 30 ppm, $A_{3,GPA}$ is set equal to $A_{S,3}$. This equivalence is also assigned in cases when the assigned sulfur level is greater than sulfurGPAmax (i.e., 330 ppm).

To calculate a combined sulfur adjustment, the values of $A_{S,3}$ and $A_{3,GPA}$ are weighted by the “GPA fraction” (f_{GPA} , GPAFract) in a county being simulated, as shown in Equation 3-14. In the default values assigned in the database, the fraction is always 0 or 1. However, GPA fraction is a user input, allowing assignment of alternate values between 0 and 1.

$$A_{S,combined} = (1 - f_{GPA})A_{S,3} + f_{GPA}A_{3,GPA} \quad \text{Equation 3-14}$$

3.2.4.6 Weighting for “Normal” and “High” Emitter Fractions

The original M6Sulf algorithm produced separate sulfur corrections for “Normal” and “High” emitters, as described in Section 3.2.2. However, because MOVES2014 does not attempt to distinguish “normal” and “high” emitter classes, the sets of model coefficients for “normal” and “high” emitters were regarded as independent models and assigned equal weights for consistency with the underlying analyses (i.e., $w_{normal} = w_{high} = 0.50$). In the database table sulfurModelCoeff, the sulfurCoeff field takes different values for “normal” and “high” emitter classes (denoted by *M6emitterID*). These calculations shown in **Equation 3-2** to **Equation 3-9** are applied to both target and base fuels, as shown in **Equation 3-15**.

$$\begin{aligned} A_{S,3}^{target} &= (1 - w_{high})A_{S,3,normal}^{target} + w_{high}A_{S,3,high}^{target} \\ A_{S,3}^{base} &= (1 - w_{high})A_{S,3,normal}^{base} + w_{high}A_{S,3,high}^{base} \end{aligned} \quad \text{Equation 3-15}$$

Likewise, a composite of normal and high emitter GPAsulf adjustments are calculated using the same weights.

$$\begin{aligned} A_{3,GPA}^{target} &= (1 - w_{high})A_{3,GPA,normal}^{target} + w_{high}A_{3,GPA,high}^{target} \\ A_{3,GPA}^{base} &= (1 - w_{high})A_{3,GPA,normal}^{base} + w_{high}A_{3,GPA,high}^{base} \end{aligned} \quad \text{Equation 3-16}$$

3.2.4.7 Computing the Sulfur Adjustment for Base and Target Fuels

During a model run, the calculations described to this point (sections 3.2.4.1 through 3.2.4.6) are repeated and applied for the two base fuels with 90 ppm and 30 ppm sulfur, corresponding to the two model-year ranges (1960-2000 and 2001-2050), respectively. This step is taken because the final sulfur fuel adjustment is the ratio of the adjustments for the target and base fuels, as shown in **Equation 3-17** for non-GPA and GPA areas. All calculations described are identical for the target and base fuels. The sulfur adjustments are calculated independent of the other fuel properties of the base fuels. A final sulfur adjustment for fuels containing 30 ppm sulfur resolves to 1.0 because the target fuel level is equal to the base fuel of 30 ppm. The 30 ppm sulfur level is called the *basis* because the entire M6Sulf algorithm was developed based on this level. The calculation result does not equal 1.0 for the 90 ppm base sulfur. As stated earlier, the M6Sulf

model applies to all sulfur levels for model year group 1960-2000, and only to sulfur levels above 30 ppm for model year groups 2001-2050.

$$A_{S,final} = \frac{A_{S,3}^{target}}{A_{S,3}^{base}}$$

Equation 3-17

$$A_{GPA,final} = \frac{A_{3,GPA}^{target}}{A_{3,GPA}^{base}}$$

3.2.4.8 Summary of Equations and Variables for M6Sulf Model

Table 3-15 provides a glossary and brief description of the variables shown in the calculations presented in Section 3.2.

Table 3-15. Glossary of Variables and Equations for calculations described in 3.2.

Eqn	Eqn(GPA)	Symbol	Name	Type (DB table)	Description
3-2, 3-3, 3-4, 3-5	3-10	β	<i>sulfurCoefficient</i>	DB input (<i>Sulfurmodelcoeff</i>)	Regression coefficient for short-term sulfur effects (log-log or log-linear).
3-2	3-10	x_S	<i>sulfurTarget</i>	DB Input (<i>FuelFormulation</i>)	“target” sulfur level for geographic region and time period covered in a MOVES run. (in Eqn 3-10 takes value of $x_{S,GPAmax}$).
3-3		$x_{S,basis}$	<i>sulfurBasis</i>	DB input (<i>SulfurBase</i>)	The base sulfur level for all calculations in MOVES run is constant at 30 ppm.
3-2, 3-4	3-10	$C_{short,target}$	Short-term correction for target sulfur level	Intermediate result	
3-3, 3-5		$C_{short,basis}$	Short-term correction for the base sulfur level	Intermediate result	
3-6	3-11	$A_{S,short}$	SulfAdj	Intermediate result	Short-term sulfur effect
3-7		$A_{S,long}$	<i>sulfurLongCoeff</i>	DB input (<i>M6SulfurCoeff</i>)	Applied to vehicles in LEV and more recent standards, for S levels > 30 ppm

3-7	3-12	A_2		Intermediate result	Adjustment combining short and long-term sulfur effects. Calculated as product of $A_{S,short}$ and $A_{S,long}$.
3-8		$x_{S,cap}$	<i>maxIRFactorSulfur</i>	DB input (<i>M6SulfurCoeff</i>)	Maximum S level for which “irreversibility effect” is calculated. Varies by specified model-year groups.
3-8		ϕ	<i>sulfurCoefficient</i>	DB input (<i>Sulfurmodelcoeff</i>)	Equal to β for T0, LEV or ULEV vehicles or γ for Tier 1 vehicles.
3-8		$A_{S,irr}$	SulfIRR	Intermediate result	“irreversible sulfur effect,” applied for vehicles in model years 2004+, for S levels > 30 ppm but less than $x_{S,cap}$.
3-9		w_{IR}	<i>sulfurIRFactor</i>	DB input (<i>M6SulfurCoeff</i>)	
3-9	3-13	$A_{S,3}$	SulfAdj3	Intermediate result	Combines short-term, long-term and irreversible S effects.
3-15	3-16	w_{high}	Weight for “high-emitter” class		Assigned constant value of 0.50, i.e., “normal” and “high” classes are equally weighted.
3-17	3-17	$A_{S,final}$	Final Sulfur adjustment	Intermediate result	Calculated with base sulfur level at 90 ppm for MY1960-2000 and 30 ppm for MY 2001-2050.

3.3 Tier 2 Low Sulfur Model (T2LowSulf)

The M6Sulf model, described above, is used in MOVES2014 to model the emission effects for gasoline fuels with sulfur content greater than 30 ppm. For 2001 and later model year vehicles operating on sulfur levels equal to or below 30 ppm, a different set of corrections, the “Tier 2 Low Sulfur Model,” based on additional data collected since the M6Sulf model was created, is used.

3.3.1 Background

Following the successful implementation of the Tier 2 sulfur standards, new research has focused on the emission reduction potential of lowering sulfur levels below 30 ppm, particularly in

vehicles employing Tier 2 and newer technologies, under the hypothesis that increased reliance on the catalytic converter would result in a higher sensitivity to fuel sulfur content. A 2005 study conducted jointly by EPA and several automakers on nine Tier 2 vehicles in support of the Mobile Source Air Toxics (MSAT) rule, found significant reductions in NO_x, CO, and HC emissions when operating on 6 ppm versus 32 ppm sulfur test fuel.²² In particular, the study found a nearly 50 percent increase in NO_x when sulfur was increased from 6 ppm to 32 ppm. Another study published in 2011 by Umicore Autocat USA examined the impact of sulfur on the catalyst efficiency during repeated FTP tests using fuels with sulfur levels of 3 and 33 ppm and observed reductions of 41 percent for NO_x and 17 percent for HC on a vehicle certified to the PZEV standard.²⁴ Both of these studies conducted testing at high and low sulfur levels after running the test vehicles through test cycles intended to purge the catalyst of the effects of prior sulfur exposure. Given the preparatory procedures related to catalyst clean-out and loading used by these studies, these results may represent a “best case” scenario relative to what may be expected under more typical driving conditions.

Nonetheless, both the MSAT²⁵ and Umicore²⁴ studies showed the emission reduction potential of lower sulfur fuel on Tier 2 and later technology vehicles over the FTP cycle. However, assessing the potential for reduction on the in-use fleet requires understanding how sulfur exposure over time impacts emissions, and what the state of catalyst sulfur loading is for the typical vehicle in the field.

3.3.2 Data Used in Developing the T2LowSulf Model

To gain further understanding of the effect of fuel sulfur on emissions, EPA conducted a study assessing the state of sulfur loading (i.e., “poisoning”) in typical in-use Tier 2 vehicles, as well as the effect of fuel sulfur level on these vehicles during subsequent mileage accumulation.²⁶ The project was designed to take into consideration what was known from prior studies on sulfur build-up in catalysts over time and the effect of periodic regeneration events that can occur during higher speed and load operation in day-to-day driving.

The test fleet was chosen to be representative of latest-technology light duty vehicles being sold at the time the program was launched. The study did not attempt to analyze or model details of after-treatment design specific to each vehicle model such as catalyst position, precious metal types and quantities used, or related engine control strategies such as timing advance at cold start or fuel cut during deceleration. While these things undoubtedly influence the behavior of emissions and may interact with the fuel sulfur effects being investigated, including them in an analysis requires correctly assessing and parameterizing them for all vehicles in the study. Instead, this program’s aim was to characterize overall effects of sulfur on emission inventories by observing the aggregate behavior of a representative fleet of vehicles.

The main and largest group of vehicles was intended to conform on average to the Tier-2/Bin-5 exhaust certification level and employ a variety of emission control technologies. These goals could be achieved by including a range of vehicle sizes, engine displacements, and manufacturers. A list of 19 high-sales-volume makes and models based on 2006-8 sales data and projections had been used for test fleet selection in the EPA/V2/E-89 study that was launched shortly before this study.⁴² Given that we would be targeting recruitment of vehicles 1-3 years old, this list seemed relevant, with the added benefit that the emission behavior of these same

models would also be characterized in the other study's results. Grouping sales data by engine family allowed additional transparency and flexibility in choosing test vehicles that represent a wider group with identical powertrains without targeting one specific make and model. The resulting target list of 19 vehicle models for recruitment is shown in Table 3-16. The vehicle sample included in the program consisted of 93 cars and light trucks recruited from owners in southeast Michigan, covering model years 2007-9 with approximately 20,000-40,000 odometer miles. While the sample for the main study did not specifically target vehicles certified to the lowest emissions standards (e.g., Bin 3, Bin 2), the supplemental study acquired additional vehicles with "Tier 3 like" emission levels and technologies, as discussed in 3.3.3.5.2.

The test fuels used were two non-ethanol gasolines with properties typical of certification fuel, with sulfur levels of 5 and 28 ppm, with the higher level chosen to represent retail fuel available to the public in the vehicle recruiting area (see Table 3-16 for detailed fuel properties). All emissions data was collected using the FTP cycle at a nominal ambient temperature of 75°F.

Table 3-16. Vehicles Targeted for Recruitment.

Model Year	Make	Brand	Model	Engine Size	Engine Family	Emissions Standard Level¹
2008	GM	Chevrolet	Cobalt	2.2L I4	8GMXV02.4025	5
2007	GM	Chevrolet	Impala FFV	3.5L V6	8GMXV03.9052	5
2007	GM	Saturn	Outlook	3.6L V6	8GMXT03.6151	5
2007	GM	Chevrolet	Silverado FFV	5.3L V8	8GMXT05.3373	5
2007	Toyota	Toyota	Corolla	1.8L I4	8TYXV01.8BEA	5
2008	Toyota	Toyota	Camry	2.4L I4	8TYXV02.4BEA	5
2007	Toyota	Toyota	Sienna	3.5L V6	8TYXT03.5BEM	5
2007	Toyota	Toyota	Tundra	4.0L V6	8TYXT04.0AES	5
2008	Ford	Ford	Focus	2.0L I4	8FMXV02.0VD4	4
2007	Ford	Ford	Taurus	3.5L V6	8FMXV03.5VEP	5
2007	Ford	Ford	Explorer	4.0L V6	8FMXT04.03DB	4
2008	Ford	Ford	F150 FFV	5.4L V8	8FMXT05.44HF	8
2007	Chrysler	Dodge	Caliber	2.4L I4	8CRXB02.4MEO	5
2007	Chrysler	Dodge	Caravan FFV	3.3L V6	8CRXT03.3NEP	8
2008	Chrysler	Jeep	Liberty	3.7L V6	8CRXT03.7NE0	5
2008	Honda	Honda	Civic	1.8L I4	8HNXV01.8LKR	5
2008	Honda	Honda	Accord	2.4L I4	8HNXV02.4TKR	5
2007	Honda	Honda	Odyssey	3.5L V6	8HNXT03.54KR	5
2007	Nissan	Nissan	Altima	2.5L I4	8NSXV02.5G5A	5
¹ Certification standard level under the Federal Tier-2 standards.						

Table 3-17. Test Fuel Properties.

Fuel Property	ASTM Method	Low S Test Fuel	High S Test Fuel¹
Sulfur	D2622	5 ppm	28 ppm
Benzene	D5769	0.34 Vol. %	0.34 Vol. %
Total Aromatics	D5769	31.2 Vol. %	31.2 Vol. %
Olefins	D1319	0.5 Vol. %	0.5 Vol. %
Saturates	D1319	68.3 Vol. %	68.3 Vol. %
Oxygenates	D5599	0.0 Vol. %	0.0 Vol. %
T50	D86	221°F	221°F
T90	D86	317°F	317°F
RVP	D5191	9.0 psi	9.0 psi
¹ Sulfur content was confirmed for the higher-sulfur test fuel, while other properties were assumed to be the same as the typical certification fuel given the small amount of dopant added.			

The data generated in this program included three distinct but overlapping datasets, designated as: “clean-out at 28 ppm,” “clean-out at 5 ppm,” and “mileage accumulation at target sulfur level.” The “sulfur level” data provide the key information for assessing the in-use effect of target sulfur levels on emissions over time as vehicles accumulated mileage. These data are the most relevant in the context of MOVES2014 and therefore, only the analyses pertaining to the “sulfur level” data are discussed in the following section. For additional details on the study design, test procedures, and the complete analyses, see the project report.²⁶

The “sulfur level” data represent the emission measurements from the repeated FTP cycles following clean-out and include all measurements from vehicles tested on “low” and “high” sulfur levels. Measurements were completed on a total of 35 vehicles representing 19 engine families (Table 3-18). The average starting odometer of the 35 vehicles was 31,178 ± 6,351 miles. A total of 322 measurements were taken – 161 measurements each for both high and low fuel sulfur levels, where a “measurement” represents a completed FTP cycle.

Table 3-18. Description of Tier 2 Vehicles in the “Sulfur Level” Dataset.

Vehicle Family ID	Vehicle ID	Make	Model	Model Year	Tier-2 Bin	Number of Vehicles	Average Starting Odometer (mi)
M500	0003	Toyota	Corolla	2007	5	1	33,122
M501	0023	Ford	Explorer	2007	4	1	27,562
M502	0026	Dodge	Caliber	2007	5	1	29,097
M503	0194	Honda	Odyssey	2007	5	1	35,816
M504	0021	Saturn	Outlook	2007	5	1	43,733
M505	0031	Chevrolet	Silverado	2007	5	1	27,891
M506	0123	Nissan	Altima	2007	5	1	39,936
M507	0148	Ford	Taurus	2007	5	1	28,802
M508	0075	Dodge	Caravan	2007	8	1	41,117
M509	0046	Chevrolet	Impala	2007	5	1	37,734
N510	0264	Toyota	Sienna	2007	5	1	38,464
N511	0179	Chevrolet	Cobalt	2008	5	1	38,722
N512	0107	Jeep	Liberty	2008	5	1	24,614
N513	0089, 0178	Ford	Focus	2008	4	2	24,726
N514	0010, 0101, 0104	Honda	Civic	2008	5	3	32,931
N515	0006, 0007, 0074, 0165	Ford	F150	2008	8	4	29,738
N520	0011, 0022, 0026,	Toyota	Tacoma	2009	5	3	28,964
N521	0131, 0162, 0179, 0280, 0329	Toyota	Camry	2008	3	5	28,506
P522	0009, 0039, 0146, 0045, 0011	Honda	Accord	2008	3	5	29,601

3.3.3 Data Analysis and Results

The pollutants included in the analysis were total hydrocarbons (THC) as reported by the FID analyzer, carbon monoxide (CO), oxides of nitrogen (NO_x), methane (CH₄), as well as particulate matter (PM) mass. Although each bag, ‘Bag 1 minus Bag 3’, and the composites from the FTP test cycle were analyzed separately in the original analysis, only the analyses and the results for Bag 2 (capturing the running emissions) and ‘Bag 1 minus Bag 3’ (capturing the cold-start emissions) are presented in this document. The statistical methodologies described in the following section were applied consistently in the analysis of all pollutants and all bags. However, the analysis of nitrogen oxides (NO_x) from Bag 2 is presented in greater detail to assist the reader in understanding the analytical approaches and to illustrate the statistical methods used.

Note that the design of the experiment and data analysis went through an independent peer-review process in accordance with EPA’s peer review policy. The results of the peer review^{27,28} largely supported the study design, statistical analyses, and the conclusions from the program

and raised only minor concerns that have not changed the overall conclusions and have subsequently been addressed in the final version of the project report.²⁶

3.3.3.1 *Data Preparation*

Prior to proceeding with the statistical analyses, issues associated with very low emissions measurements and outlying observations were examined. The following sections describe how these issues were addressed.

3.3.3.2 *Imputation of Measurements with Low Concentration*

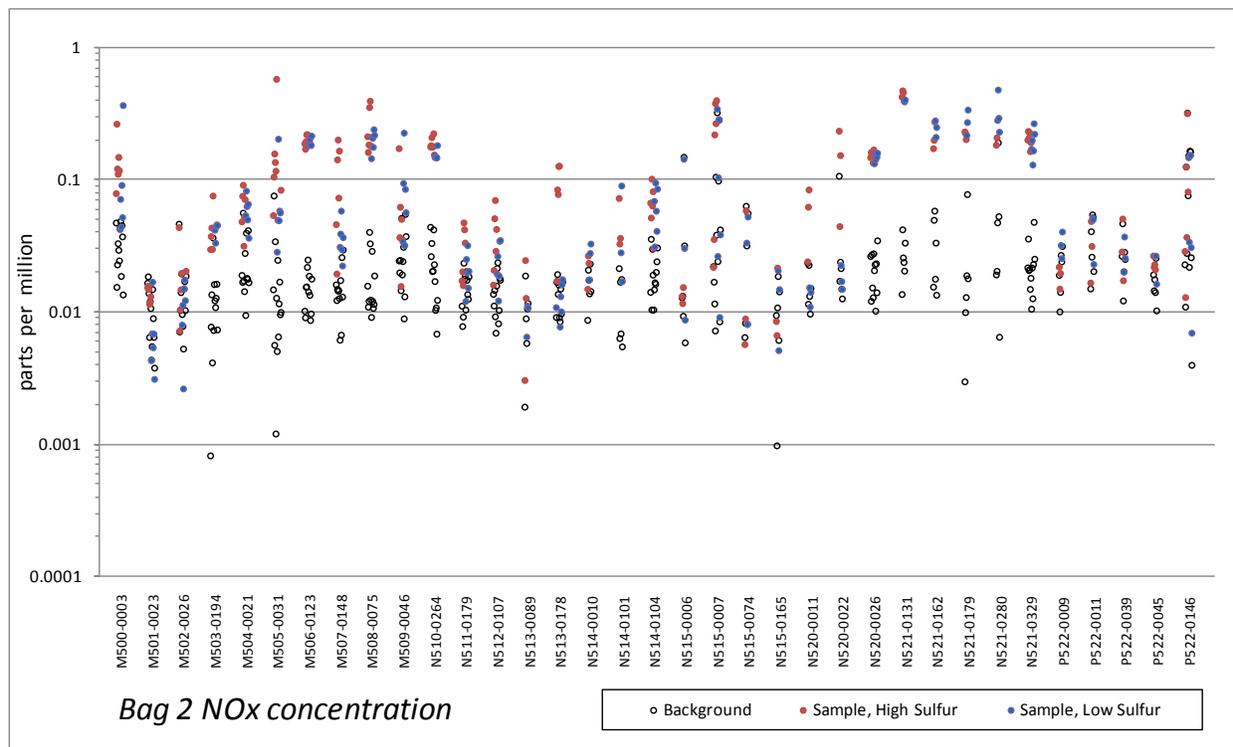
The graphical examination of the “sulfur level” dataset revealed the presence of very low emission measurements from some pollutants and bags including NO_x Bag 2. Since uncertainty associated with these low measurements could potentially affect the outcome of the analysis, it was important to understand the measurement process and evaluate the impact of associated uncertainties.

During emissions testing, the vehicle exhaust stream was collected and diluted with background air to avoid condensation of water vapor and other factors affecting the stability of the chemical species. A small sample of this mixture flows into a collection bag for analysis after the test. The concentration of emission species in the bag is determined by flowing the contents through a properly-calibrated gas analyzer. This method provides a time-weighted result via physical integration of the emission stream produced over the course of a transient driving cycle.

Uncertainty in the measurement process results from the physics of mixing and sampling from a gas stream as well as “noise” in analyzer components such as optoelectronic detectors and signal amplifiers. This presence of these factors means that repeated measurements taken under identical process conditions will produce a range of results, their average being the true (intended) response of the instrument and the range around it representing the measurement variability.

For the analyzers used in this program, the size of the measurement error (in relative terms) is expected to increase relative to the measured value as the concentration decreases. Moreover, the dilute-bag method used requires measurement of concentrations in both sample and background bags, followed by a subtraction between the two, such that the net result contains variability from both measurements. To assess whether these issues affected this dataset, we examined plots of the measured concentrations for each test by vehicle by pollutant and bag. Figure 3-1 shows the Bag 2 NO_x dataset for the vehicles providing the “sulfur level” data, which contains a number of very low values, as well as tests where sample and background are of similar magnitude (the vehicle codes refer to the Family IDs listed in Table 3-18. Given these findings, we performed sensitivity analyses to evaluate the impact of these low emission measurements on the study results (presented in 3.3.3.5.3).

Figure 3-1. NO_x (Bag 2): Concentrations for Hot-running Emissions by Vehicle.



When a dilute emission measurement is lower than the measured background level, the net result is reported as zero (this calculation is performed on a test-by-test basis). However, as it is unlikely that tailpipe emissions are truly zero during a test, it was assumed that a “zero” result indicates that the actual emissions level was smaller than the sum of the measurement errors occurring on the sample and background measurements. The emission level was thus considered to be below the limit of quantitation (LOQ), a level below which we are not confident in the accuracy of quantitative values.

In this situation, the data point can be assigned a value of zero, deleted, or replaced with an imputed value. However, because it was necessary to apply a natural log-transformation, zero values were not retained in the data. Table 3-19 summarizes the number of measurements with zero values, with percentages in parentheses. Given that observations below the LOQ appear to be randomly distributed across sulfur levels and vehicles, and since excluding such observations would result in reduced sample size, less statistical power, and larger standard errors,²⁹ they were imputed in the analysis.

Since an imputation method involving each vehicle’s own longitudinal data would be superior to methods using no information about the vehicle,³⁰ a commonly-used single-imputation method, using half the minimum of a valid measurement from a given mileage bin for the vehicle with zero values, was performed. This imputation method recognized the fact that emission measurements below the limit of quantitation must be smaller than any quantified value.

Since vehicle-specific imputation which minimizes the likelihood of artificially reducing the natural variance of the data was used and the numbers of measurements with imputed values are less than 20 percent (Table 3-19), we can expect good estimates of the reliability of measurements.³¹ Nonetheless, it is important to determine the effect of these imputed values on the resulting test statistics and corresponding conclusions. Thus, the results from the statistical analysis with and without the imputed values were compared once the model was finalized to assess the potential for introducing bias.

Table 3-19. Numbers of Measurements with Zero Values in Sulfur Level Data

	NO_x	THC	CO	PM
Bag 2	21 (6.5%)	14 (4.3%)	10 (3.1%)	2 (0.9%)
Bag 1 – Bag 3	7 (2.2%)	0	1 (0.3%)	15 (6.5%)

3.3.3.3 *Detection of Outliers*

Prior to proceeding to the full analysis, preliminary models were fit to detect extreme values or “outliers.” The residual plots were visually inspected for outlying observations and the outliers were identified using the screening criterion value of ± 3.5 for the externally studentized residuals. Generally, one can expect about 95% of the externally studentized residuals to be within ± 3.5 standard deviations. This criterion has been widely used in statistics. When the outlying observation represented an actual measurement, it was examined to assess its validity. Since none of the outliers representing actual measurements showed clear indications of measurement error, it was assumed that the outlying observations were valid and thus they were included in the dataset for analysis. However, there were instances where a very low imputed value was identified as an outlier. In such instances, the imputed values were removed from the dataset. Table 3-20 summarizes the numbers of outliers as well as numbers of imputed measurements removed (in parentheses).

Table 3-20. Number of Outliers in Sulfur Level Data (Numbers of Imputed Values removed).

	NO_x	THC	CO	PM
Bag 2	0 (0)	1 (1)	4 (1)	1 (0)
Bag 1 – Bag 3	2 (0)	2 (0)	6 (1)	4 (0)

3.3.3.4 *Modeling Methodology*

The following section describes the statistical approaches and the model-fitting methodologies applied in the analysis. First, the emission measurements were log-transformed. In the current

study, the distributions of emissions exhibited positive skewness (log-normal), and thus, transforming emission measurements by the natural logarithm was necessary to stabilize the variance, to obtain a linear relationship between the mean of the dependent variable and the fixed and random effects, and to normalize the distributions of residuals. The log-transformation of emission measurements has been well-established in previous studies analyzing vehicle emissions data.^{32,33,34}

The “sulfur level” data is a classic example of “repeated measures data” where multiple measurements were taken on a single vehicle at different accumulated mileages. The conventional methods for analyzing “repeated measures data” are the univariate and multivariate analysis of variance. However, the linear mixed model was selected for the analyses of the “sulfur level” data for the following reasons: The mixed-model approach uses generalized least squares to estimate the fixed effects, which is considered superior to the ordinary least squares used by the univariate and multivariate procedure.³⁴ It is a more robust and flexible procedure in modeling the covariance structures for repeated measurements data and better accounts for within-vehicle mileage-dependent correlations.^{32,33} In addition, the mixed model is capable of including vehicles with missing data and handling irregularly spaced measurements.

The MIXED procedure in the SAS 9.2 software package was used to fit the model. The mixed model is represented in Equation 3-18 as:

$$Y_i = X_i\beta + Z_iu_i + \varepsilon_i \quad \text{Equation 3-18}$$

where β and u_i are sets of fixed and random effects parameters, respectively, and ε_i is a set of random residuals. The mixed model accounts for correlation in the data through the inclusion of random effects and modeling of the covariance structure. The set of fixed-effect coefficients β represent the mean effects of sulfur level across the set of measured vehicles and the set of random coefficients u_i represent parameters (i.e., slopes or intercepts) allowed to vary by vehicle, reflecting the natural heterogeneity in the measured fleet. In other words, the model incorporates differences in the effect of sulfur level on emissions from individual vehicles. The distributional assumptions for the mixed model are: u_i is normal with mean 0 and variance G_i ; ε_i is normal with mean 0 and variance R_i ; the random components u_i and ε_i are independent.

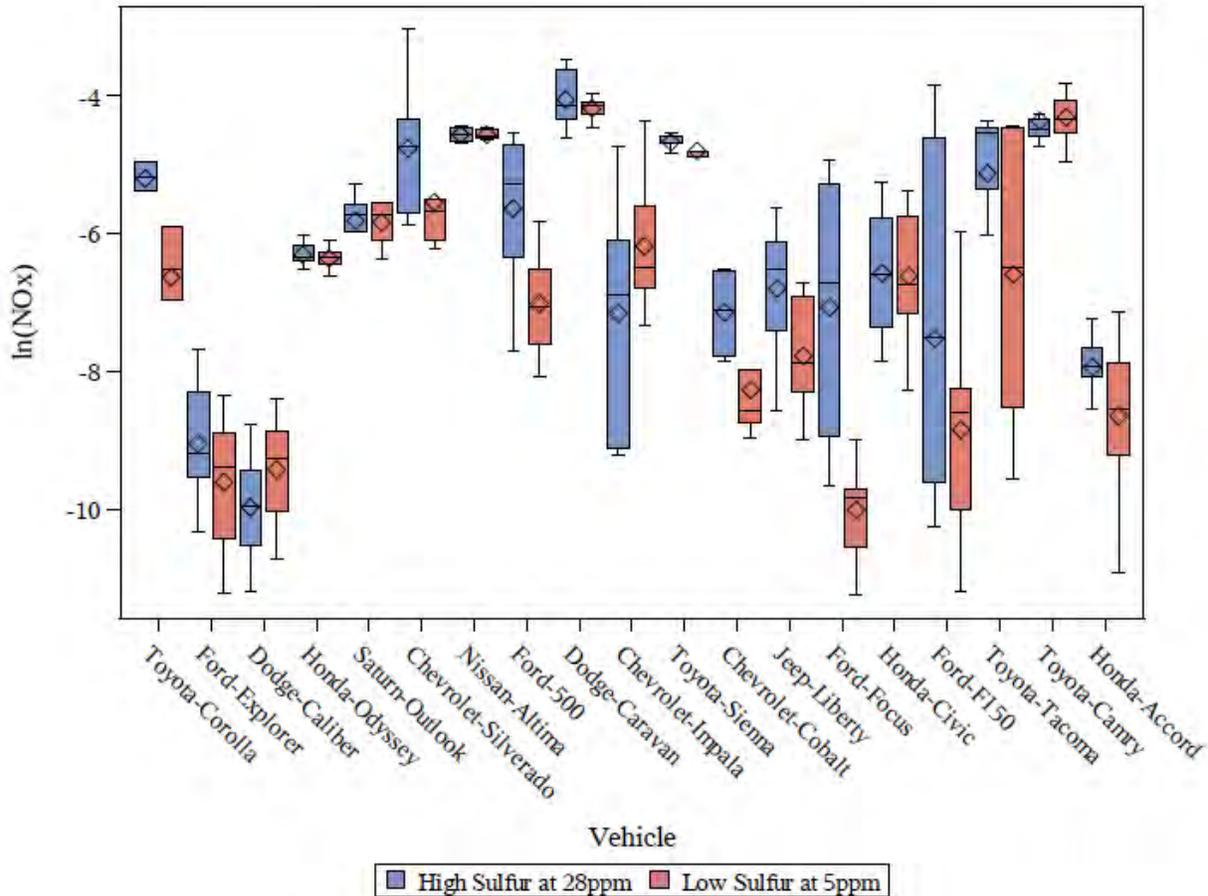
In developing the mixed model, a top-down model fitting strategy was used, similar to previously established methods.^{35,36} The first step was to start with a “saturated” or full model, which included all candidate fixed effects to allow unbiased estimation of the random effect estimates. Next, we selected an optimal covariance structure, which specifies the variation between vehicles as well as the covariation between emission measurements at different accumulated mileages on the same vehicle. Finally, the fixed-effects portion of the model was reduced to fit the final model.

3.3.3.5 Statistical Analysis and Results

3.3.3.5.1 Tier 2 Vehicles

The box-plot of the log-transformed emissions from Bag 2 NO_x “sulfur level” data (Figure 3-2) shows the spread of the data for each vehicle family and sulfur level across all mileages. The diamond and the line inside the box represent the mean and the median, respectively. The box represents the interquartile range between 25th and 75th percentile and the error bars show the full data range. Generally, there is a tendency for the vehicles running on high sulfur fuel to emit more NO_x than the vehicles running on low sulfur fuel. However, the effect of operation on higher sulfur fuel certainly varies by vehicle family, suggesting the presence of substantial between-vehicle family variability. For example, the Toyota Corolla, Ford Focus, and Chevrolet Cobalt clearly show a large effect of fuel sulfur level on emissions while the effect is more marginal for the Nissan Altima and Honda Civic.

Figure 3-2. Box-Plot of Individual Vehicle Families by Sulfur Level (NO_x Bag 2).

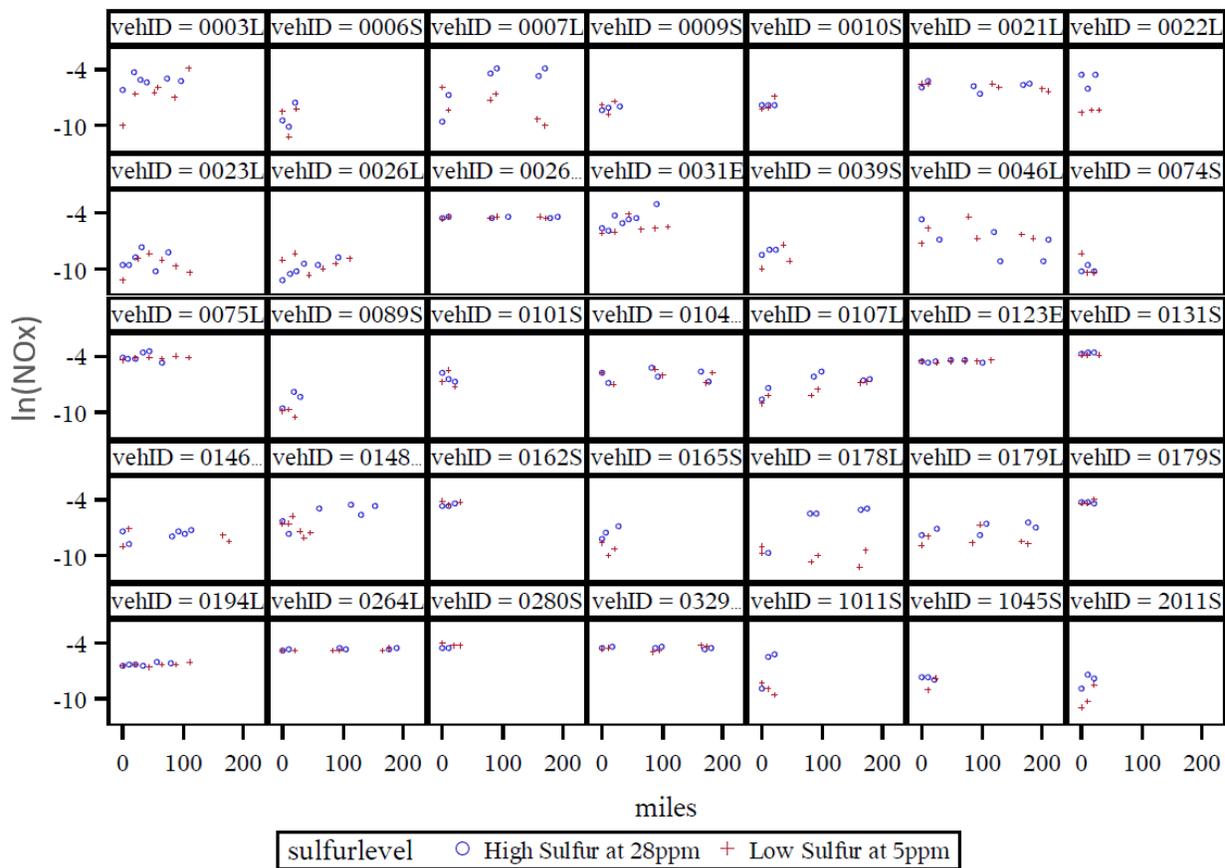


In the dataset, the numbers of tested vehicles are not the same across vehicle families. Considering the differences in numbers of unique vehicles in each vehicle family and the presence of variability among vehicle families illustrated in Figure 3-2, each vehicle family was considered as a random effect in constructing the statistical model.

Figure 3-3 presents the ln-transformed emissions from individual vehicles by sulfur level. The plot shows that the increase in emissions as vehicles accumulate mileage for the high sulfur level is more significant compared to the low sulfur level, contributing to the increased variance for some vehicles and suggests that the rate of sulfur loading might differ for the two sulfur levels. Thus, an interaction between sulfur level and the accumulated mileage was included in the statistical modeling of the data. Thus, these findings from the graphical examination of the data assisted in formulating the statistical models fit to the data.

We refrained from looking at the simple descriptive statistics, such as means and standard deviations, to assess the relationship between the sulfur level and emissions even as a preliminary step, because reaching conclusions from such naïve approaches can be very misleading as they fail to account for such factors as the presence of repeated measurements and variability both between and within vehicles. In addition, the mileage accumulations varied from vehicle to vehicle, and simple descriptive statistics would not capture the substantial degree of variability inherent in the dataset.

Figure 3-3. Log-Transformed Emissions from Individual Vehicles by Sulfur Level (NO_x Bag 2).



In analyzing the “sulfur level” data, a top-down model fitting approach was applied to characterize the effects of fuel sulfur level on emissions as a function of accumulated mileages

since cleanout. The dependent variable (Y_i) was the natural logarithm of emissions. The fixed effects (X_i) included in the model were sulfur level, accumulated mileage, vehicle type, and the interaction terms. The random effects (Z_i) were each vehicle family in the study. The likelihood ratio test for the significance of between-vehicle variation was statistically significant for all pollutants and bags, and thus, the random intercept for each vehicle family was included in the model. The significance of the between-vehicle variation was observed graphically in Figure 3-3.

All measurements from the same vehicle family were assigned the same between-vehicle family error variance; their within-vehicle family error variances will differ, and can be correlated within a vehicle family. The measurements from the same vehicle family are assumed to be correlated because they share common vehicle characteristics and have similar emission profiles. Also, measurements on the same vehicle close in time are often more highly correlated than measurements far apart in time as observed in Figure 3-3 – the covariation within vehicles. Both within- and between-vehicle errors are assumed independent from vehicle to vehicle. Since the measurements on different vehicles are assumed independent, the structure refers to the covariance pattern of measurements on the same subject. For most of these structures, the covariance between two measurements on the same vehicle depends only on the differences in mileage accumulation between measurements, and the variance is constant over mileage.

The covariance structure was modeled by first fitting the “unstructured” (UN) covariance matrix with a saturated model including all fixed effects, which failed to converge. Next, since emissions were measured irregularly, where the mileage intervals between measurements are more or less unique to each vehicle, the spatial covariance structure, which allows for a continuous representation of mileage, was fit. However, the model failed to converge for the spatial covariance matrix as well. Thus, we proceeded to fit the compound symmetry (CS) structure which specifies that measurements at all mileages have the same variance, and that all measurements on the same vehicle have the same correlation. The Bayesian Information Criterion (BIC) value for the compound symmetry was 803.36.

Lastly, the first-order autoregressive structure (AR1) was modeled. This structure assumes that the variances are homogeneous and the correlations decline exponentially with time, i.e., the error variance in measured emissions is constant for all vehicles at all mileage levels, and sets of measurements close in time (i.e., mileage) are more highly correlated than the measurements further apart. The BIC value for the first-order autoregressive structure was 764.90. Since the BIC value for the first-order autoregressive structure was lower than that for compound symmetry, the autoregressive structure (Equation 3-19) was selected to model the covariance structure of the residuals.

$$R_i = Var(\epsilon_i) = \begin{bmatrix} \sigma^2 & \sigma^2 \rho & \sigma^2 \rho^2 & \dots & \sigma^2 \rho^{n-1} \\ \sigma^2 \rho & \sigma^2 & \sigma^2 \rho & \dots & \sigma^2 \rho^{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sigma^2 \rho^{n-1} & \sigma^2 \rho^{n-2} & \sigma^2 \rho^{n-3} & \dots & \sigma^2 \end{bmatrix} \quad \text{Equation 3-19}$$

where:

σ^2 = variance,

ρ = correlation between measurements,

n = number of measurements

A combination of first-order autoregressive structure within vehicles and a random effect between vehicles was used to model the covariance structure which specified an inter-vehicle random effect for differences between vehicles, and a correlation structure within vehicles that decreases with increasing mileage lag between emission measurements. Furthermore, the error variance associated with the low sulfur level was permitted to differ from the variance associated with the high sulfur level. Since the first-order autoregressive structure was selected due to limited available options, we acknowledge that there might be some limitations inherent in the assumption of constant distance between two measurements. However, the estimates of fixed effects, such as the differences between sulfur level means, may be the same for different covariance structures, differing only in the standard errors of these estimates.

Once the structures for the random effects and the covariance structure for the residuals were selected, the fixed effects in the model were tested using the approximate F -test with the Satterthwaite approximation for denominator degrees of freedom. The step-wise backward elimination approach was used to remove any non-significant fixed effects (shown in red in Table 3-21), starting with the saturated model. The significance level of 10% ($\alpha = 0.1$) was used to test the null hypothesis while keeping statistical hierarchy.

Table 3-21. Type 3 Tests of Fixed Effects (NO_x Bag 2)

Model	Effect¹	Num DF	Den DF	F Value	Pr > F[‡]
Model 1	slevel	1	254	7.66	0.0061
	miles	1	271	0.10	0.7499
	vehclass	1	18.2	0.18	0.6761
	slevel * miles	1	170	0.79	0.3743
	miles * vehclass	1	280	1.20	0.2748
Model 2	slevel	1	259	7.63	0.0062
	miles	1	264	17.07	< 0.0001
	vehclass	1	17	0.40	0.5363
	slevel * miles	1	175	0.72	0.3982
Model 3	slevel	1	259	7.66	0.0061
	miles	1	264	17.08	< 0.0001
	slevel * miles	1	174	0.70	0.4028
Model 4	slevel	1	219	18.28	< 0.0001
	miles	1	270	17.54	< 0.0001

¹ slevel = sulfur level (high and low); miles = accumulated mileage since clean-out;
vehclass = vehicle types (car and truck); [‡] Pr > F represents the p-value associated with the F statistic.

Finally, a likelihood-ratio test was performed to examine if the model could be reduced further without compromising the model fit. For example, in comparing model 4 and 5 (Table 3-22), the result of the likelihood ratio test was not statistically significant, we concluded that accumulated mileage does not have an effect on Bag 2 NO_x, and thus, model 5 was selected as the final model.

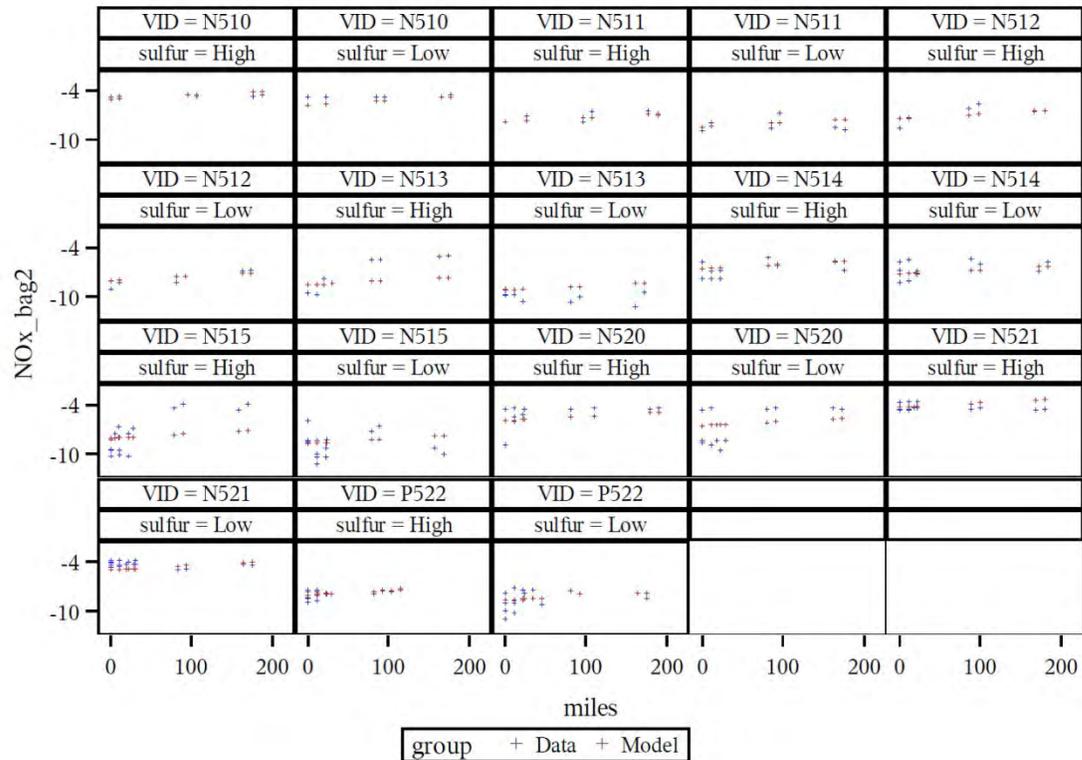
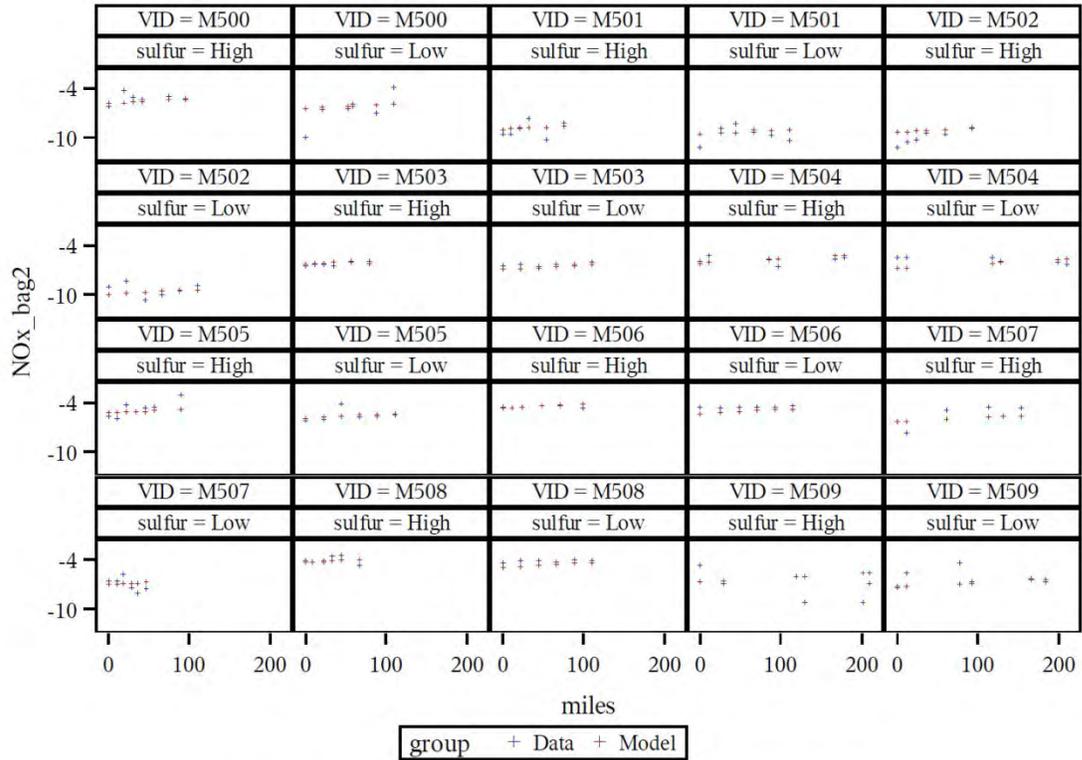
Table 3-22. Likelihood Ratio Test for Bag 2 NO_x Model.

	Fixed effects	-2 Res Log Likelihood	p-value (χ^2)
Model 4	slevel, miles	991.6	0.1213
Model 5	slevel	994	

The final NO_x Bag 2 model (model 5) retains sulfur level as the sole fixed effect. Thus, the model finds a statistically significant difference in emissions between high and low fuel sulfur levels. In addition, the sulfur effect does not differ between vehicle types (car vs. truck) as the sulfur-level × vehicle type interaction term was not significant. Also, since the mileage term is not significant, it can be concluded that the mileage accumulation after the clean-out does not increase emissions independent of the fuel sulfur level in the current analysis. In addition, since the sulfur level and the accumulated mileage interaction term was not significant, the model suggests that the rate of sulfur loading does not vary by accumulated mileages after the clean-out (up to 200 miles under the modified Long procedure) between high and low fuel sulfur levels. In other words, the effect of high fuel sulfur on Bag 2 NO_x exists immediately after clean-out and remains essentially constant on a percentage basis, during subsequent driving of a vehicle.

Figure 3-4 shows the data vs. predicted plots based on the final model for NO_x Bag 2. There are two paired plots next to each other with the same vehicle ID showing emissions from both high and low sulfur. There are some instances (e.g., VID M502) where the model overestimates the effect of sulfur by over-predicting the emission levels of high sulfur and under-predicting the emission levels of low sulfur. In contrast, there are other instances (e.g., VID M513) where the model underestimates the effect of sulfur by under-predicting the emission levels of high sulfur and over-predicting the emission levels of low sulfur. However, this is to be expected given the variability in the emission testing. In general, the model predictions are in agreement with the data.

Figure 3-4. Data vs. Predicted by Vehicle (Log-Transformed Bag 2 NO_x).



Furthermore, the one-to-one plot of data vs. model predictions in Figure 3-5 shows that the points generally lie close to the 1:1 line. In addition, the model fit has an adjusted R^2 of 0.71, demonstrating reasonable accuracy in model predictions for Bag 2 NO_x .

Figure 3-5. Data vs. Predicted (Log-Transformed NO_x Bag 2).

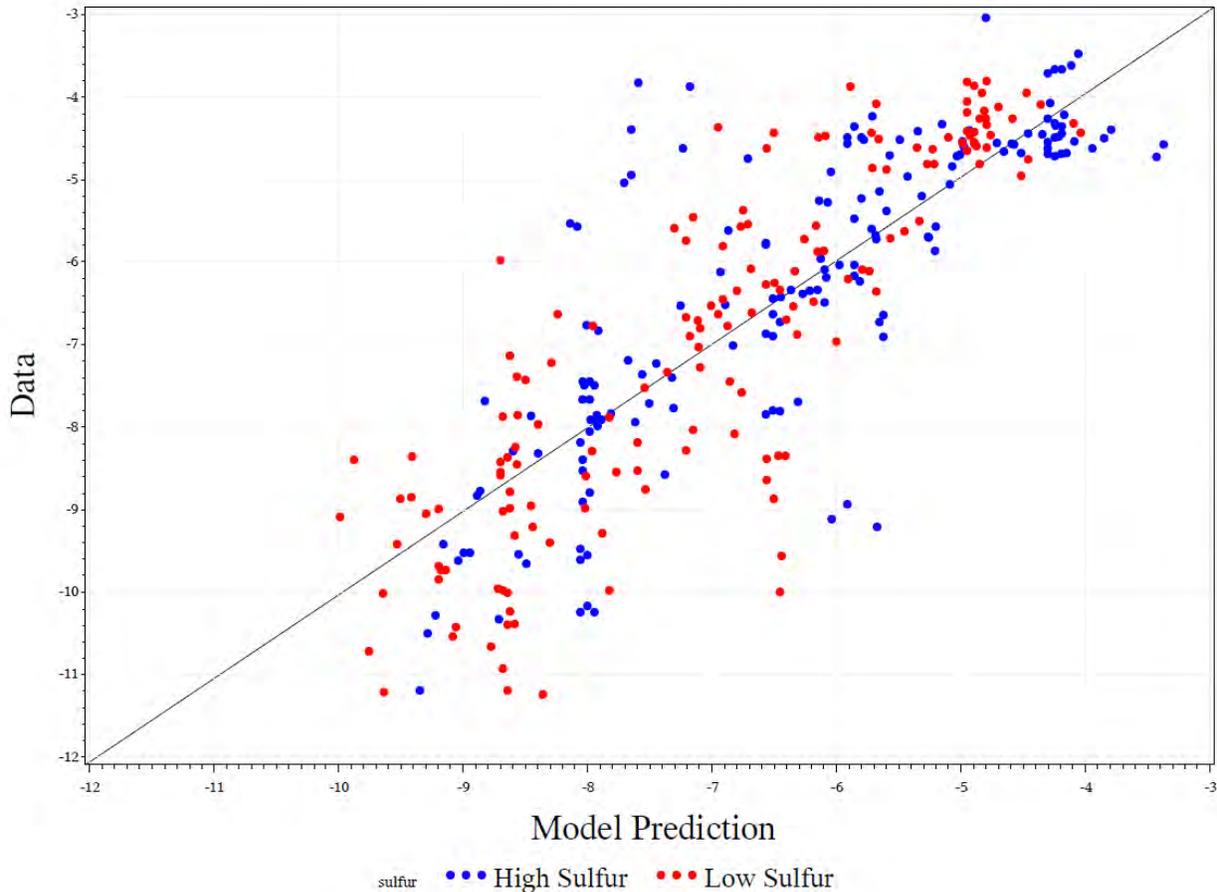


Table 3-23 summarizes the final models selected for all pollutants and bags, applying the same statistical methodology described for Bag 2 NO_x . For all models, the sulfur-level and mileage interaction terms were not significant, and the change in emissions from reducing the fuel-sulfur from 28 ppm to 5 ppm was estimated using the differences of least-squares means from the final model, adjusting for other effects in the model, using a Tukey-Kramer adjustment in calculating the p -values for the least squares means. The differences of least-squares means between high and low fuel-sulfur level were reverse-transformed to estimate the percent reduction in emissions (Table 3-24). When the sulfur level and mileage interaction term is not significant, the percent differences in emissions between high- and low fuel-sulfur levels are constant across accumulated mileage after clean-out (the sulfur loading curves for high and low sulfur are parallel) and thus, using the least squares means to quantify the reduction in emissions without considering the as-received in-use sulfur loading was sufficient.

Table 3-23. Final Selected Models for All Pollutants

Pollutant	Bag	Fixed Effects¹
NO _x	Bag 2	slevel
	Bag 1 – Bag 3	-
THC	Bag 2	slevel, miles
	Bag 1 – Bag 3	slevel
CO	Bag 2	-
	Bag 1 – Bag 3	-
PM	Bag 2	-
	Bag 1 – Bag 3	-
¹ slevel = sulfur level (high and low); miles = accumulated mileage since clean-out.		

Table 3-24 summarizes the percent reduction in emissions from the analysis for NO_x, THC, CO, and PM, which are the most relevant pollutants in the MOVES context. The percent reductions were estimated for the complete dataset with all Tier 2 standard levels included, and for a dataset including only the vehicles certified to Tier 2 Bin 8. The *p*-values represent the statistics for fuel sulfur level from the Type III *F* test. Unlike the gaseous pollutants, there was no effect of sulfur level found for PM. A plausible explanation is that the majority of PM as measured in this program (that is, from normal-emitting Tier 2 vehicles operated at low and moderate loads) was soot produced shortly after cold start (bag 1)³⁷, and the destruction of soot by the catalyst may be minimal regardless of its relative efficiency. As a result, sulfur would not be expected to have a significant effect on directly-emitted PM (other than very small amounts of sulfate). Since there were no analyses of PM composition in this program, we are not able to draw more definitive conclusions.

Table 3-24. Percent Reduction in Emissions from 28 ppm to 5 ppm Fuel Sulfur on In-Use Tier 2 Vehicles

Tier 2 Bin	Process	Pollutant			
		NO _x (<i>p</i> -value)	THC (<i>p</i> -value)	CO (<i>p</i> -value)	PM
B4, B5, B8	Hot-running ¹	51.9% (< 0.0001)	43.3% (< 0.0001)	–	–
	Cold Start ²	–	5.9% (0.0074)	–	–
B8 only	Hot-running ¹	66.3% (0.0751)	36.8% (< 0.0001)	22.1% (0.0061)	–
	Cold Start ²	–	–	–	–

¹ Measured on the hot-running Phase of the FTP cycle (Bag 2).

² Measured as the difference between the cold-start and hot-start phases on the FTP cycle (Bag 1 – Bag 3).

3.3.3.5.2 Tier-3 Equivalent Vehicles

Following the main test program with Tier 2 vehicles, a set of vehicles meeting lower “Tier- 3 equivalent” emissions standards were tested to evaluate the effect of sulfur on these newer and cleaner vehicles. These vehicles were tested using the same fuel and test procedures described earlier. The “sulfur level” data for for this subset of vehicles consisted of all measurements from the five vehicles tested on both 28 and 5 ppm sulfur fuels. A total of 64 measurements were taken – 33 measurements from high fuel sulfur levels and 31 measurements from low fuel sulfur levels. The description of the vehicles tested in the supplemental program is shown in Table 3-25.

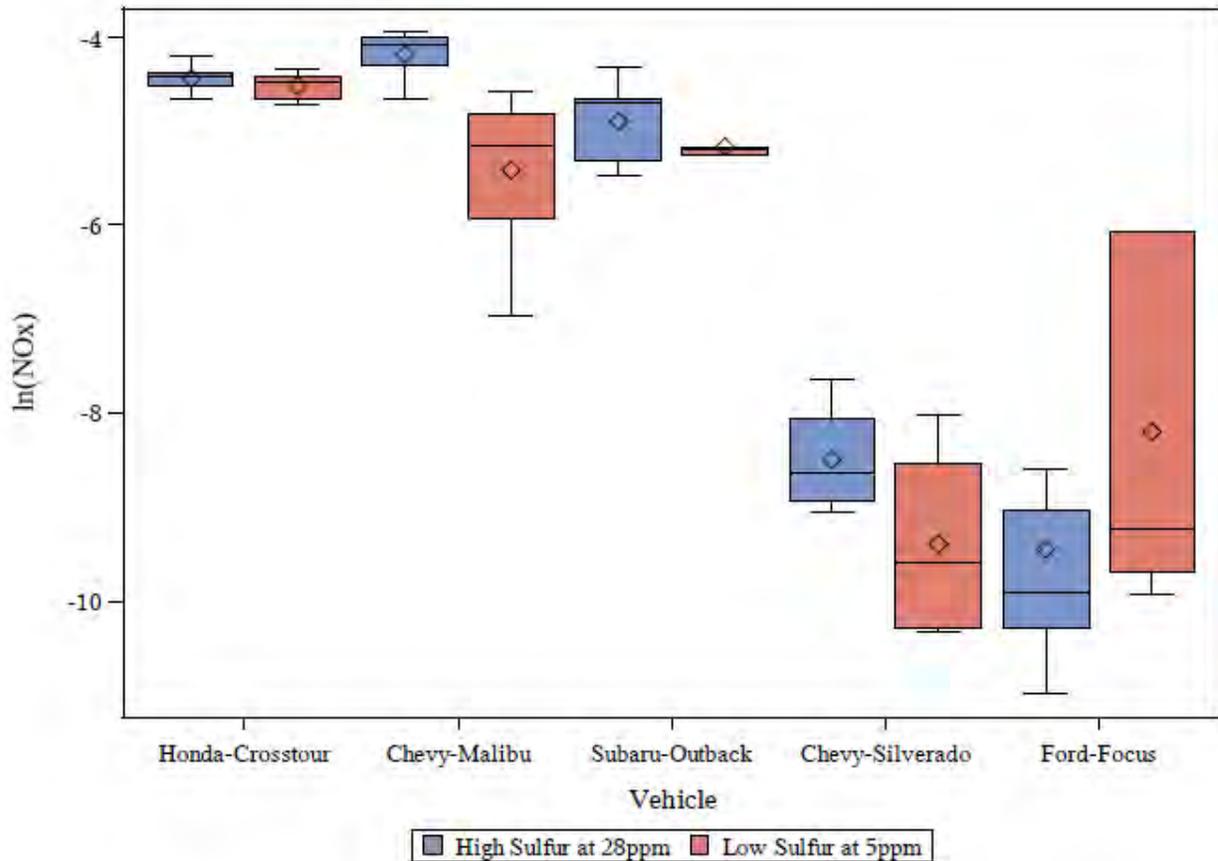
Table 3-25. Description of “Tier 3-like” Vehicles in the “Sulfur Level” Data

Vehicle Family ID	Vehicle ID	Make	Model	Model Year	Emission Standards	Starting Odometer	Vehicle Origin
P528	0001L	Honda	Crosstour	2011	ULEV	12,827	Recruited
P530	0001	Chevy	Malibu	2010	SULEV	10,285	Manufacturer ¹
P531	0001L	Subaru	Outback	2008	SULEV	36,635	Recruited
R532	0001L	Ford	Focus	2010	SULEV	28,673	EPA-owned
P532	0001L	Chevy	Silverado	2011	T2 B4	714	EPA-owned

¹ This vehicle was loaned by Umicore Autocat USA, and is the same vehicle used in their 2011 study.

The box-plot of the log-transformed emissions from Bag 2 NO_x “sulfur level” data (Figure 3-6) shows the spread of the data for each vehicle and sulfur level across all mileages. The diamond and the line inside the box represent the mean and the median, respectively. The box represents the interquartile range between 25th and 75th percentile and the error bars show the full data range. Generally, there is a tendency for the vehicles running on high sulfur fuel to emit more NO_x than the vehicles running on low sulfur fuel. However, the effect of operation on higher sulfur fuel certainly varies by each vehicle.

Figure 3-6. Box-Plot of “Tier 3-Like” Vehicles by Sulfur Level (Bag 2 NO_x).



In analyzing the “sulfur level” data for “Tier-3 equivalent” vehicles, a similar top-down model fitting statistical approach to that described earlier was applied to characterize the effects of fuel sulfur level on emissions as a function of accumulated mileages since cleanout. The dependent variable (Y_i) was the natural logarithm of emissions. The fixed effects (X_i) included in the model were sulfur level, accumulated mileage, vehicle type, and the interaction terms. The random effects (Z_i) were random intercepts for each vehicle in the study. A combination of first-order autoregressive structure within vehicles and a random effect between vehicles was used to model the covariance structure which specified an inter-vehicle random effect of differences between vehicles, and a correlation structure within vehicles that decreases with increasing mileage lag between emission measurements. The same statistical methodologies utilized for evaluating the sulfur level effects for Tier 2 vehicles were applied to these vehicles.

Table 3-26 compares the percent reduction in emissions from 28 ppm to 5 ppm fuel sulfur for Tier 2 vehicle and “Tier-3equivalent” vehicles. The results suggest that significant reductions in emissions can be achieved by reducing the fuel sulfur levels from 28 to 5 ppm in the in-use fleet of “Tier-3equivalent” vehicles. Furthermore, it shows that the cleaner vehicles are more sensitivity to the fuel sulfur levels for NO_x and CO than what was observed in the analysis of the Tier 2 vehicles. This is not unexpected since the cleaner vehicles tend to rely more on efficient catalyst activity sooner in the operation of the vehicle following the cold start. The sulfur hinders the catalyst from performing at optimal efficiency levels early in running operation, resulting in a larger penalty to these cleaner vehicles that rely more heavily on the catalyst to meet the lower emission standards. Overall, we expect lower-emitting Tier 3 vehicles to show similar or greater sensitivity to the fuel sulfur levels compared to the conventional Tier 2 vehicles.

Table 3-26. Percent Reduction in Emissions from 28 ppm to 5 ppm Fuel Sulfur for Tier 2 and “Tier 3-Like” Vehicles.

Vehicle Sample	Pollutant			
	NO _x (p-value)	THC (p-value)	CO (p-value)	PM
Tier 2 Vehicles	14.1% (0.0008)	15.3% (< 0.0001)	9.5% (< 0.0001)	–
“Tier-3 equivalent” Vehicles	23.9% (0.0203)	14.6% (0.0312)	21.0% (< 0.0001)	–

¹ Measured on the hot-running Phase of the FTP cycle (Bag 2).

² Measured as the difference between the cold-start and hot-start phases on the FTP cycle (Bag 1 – Bag 3).

3.3.3.5.3 Sensitivity Analysis

A series of sensitivity analyses of the “sulfur level” data was performed to address some of the issues that might affect the mixed-model results. They include the impacts of: measurements at very low concentrations, censoring of measurements with zero values, and influential vehicles. The sensitivity analyses were conducted only for Bag 2 NO_x, since above mentioned issues pertain the most to Bag 2 NO_x. For example, Bag 2 NO_x showed a higher percentage of measurements with zero values than most other pollutant and bag combinations.

Effect of Measurements at Low Concentration

The issue of measurements with very low concentration from Bag 2 NO_x has been discussed in 3.3.3.2. To address the uncertainty of measurements from these very low-emitting vehicles, we performed sensitivity analyses using two measurement concentration screening levels: 100 ppb (based on the lower end of the instrument manufacturer’s stated calibration range for the emission analyzer), and 50 ppb (chosen at half the former limit). In each analysis, the vehicles with all sample measurements falling below the screening level were removed, and models were re-fit. Results of these sensitivity analyses are provided in Table 3-27.

Table 3-27. Results of Sensitivity Analysis of Low Concentration Measurements (Bag 2 NO_x)

Model Description	No. of Vehicles	No. of Observations	Estimated Reduction
Final Model	35	322	51.9%
50 ppb vehicle screen	28	263	48.4%
100 ppb vehicle screen	19	191	48.2%

In each of these sensitivity analyses, the sulfur level effect remained highly significant with p -value < 0.004 , suggesting a meaningful sulfur effect exists regardless of the removal of lowest-emitting vehicles. Thus, we conclude that the sulfur effect is considerably larger than the uncertainty or error associated with the measurements.

Effect of Use of Imputed Values

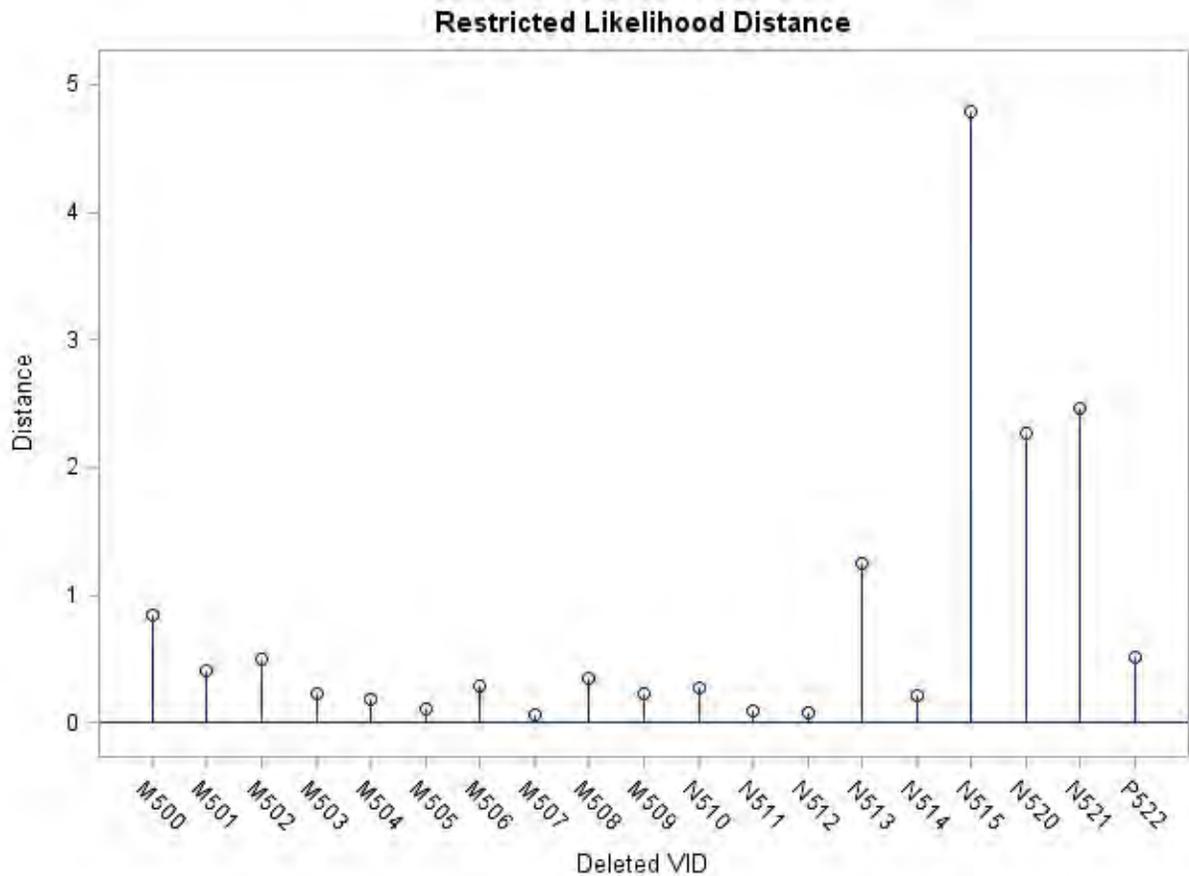
In order to assess the impact of substituting for censored values, models with and without imputed values for Bag 2 NO_x were compared. For the model without imputed values, the mixed model was re-fit using a new dataset with all imputed values removed, consisting only of actual measurements. Based on the examination of the estimates of fixed effects and the standard errors from both models, we concluded that the imputed values did not significantly bias the results. The percent reduction in emissions from 28 ppm to 5 ppm fuel sulfur level was changed from 51.9% in model with imputed values to 50.0% in model without them. The sulfur level effect remained highly significant with p -value < 0.0001 for the model with and without the imputed values.

Effect of influential vehicles

As an additional test of robustness, we also looked at the impact of removing the influential vehicles from the dataset. Influence can be broadly defined as the ability of a single or multiple vehicles to affect the resulting outcome through the presence or absence in the data. The influential vehicles can be identified by examining the restricted likelihood distance (RLD), which is calculated after an iterative process of refitting the model with and without each vehicle.

Figure 3-7 shows the restricted likelihood distance from the influence diagnostics where vehicle family IDs N515, N520, and N521 can be considered influential vehicles affecting both the fixed effects and covariance parameter estimates based on Cook's D and COVRATIO estimates. Although we do not have specific grounds for excluding these vehicles from the mixed model analysis since the measurements from these vehicles did not fall into the category of either low concentration measurements or the outlying observations, these influential vehicles were removed and the model for Bag 2 NO_x was re-fit to assess the impacts of these vehicles.

Figure 3-7. Influence Diagnostics for Bag 2 NO_x.



The resulting model showed that the percent reduction in emissions from 28 ppm to 5 ppm was 52.1 percent, compared to the reduction of 51.9 percent from the final model. This analysis demonstrated that even when the influential vehicles are removed from the analysis, the reduction in emissions from reducing the fuel sulfur level from 28 ppm to 5 ppm is still highly significant with p-value <0.0001. The sensitivity analyses examining the influential vehicles for all pollutants and bags are presented in Appendix F of the project report.

3.3.4 Application in MOVES

The results shown in Table 3-24 (page 48) were incorporated into MOVES2014 and were applied to model year 2001-and-later gasoline vehicles to estimate the sulfur effects when modeling fuel sulfur levels at or below 30 ppm. The decision to apply the results from the study of Tier 2 vehicles to model years as early as 2001 was based on the assumption that NLEV vehicles are more similar to upcoming Tier 2 vehicles than to Tier 1 vehicles.

The T2LowSulf model is applied multiplicatively in conjunction with other gasoline fuel effects in MOVES, and applies only for sulfur levels equal to and below 30 ppm. For sulfur levels above 30 ppm, and for all pre-2001 model year vehicles, the M6Sulf model is applied, as described in Section 3.2.

Equation 3-20 shows the generic form of the calculation of the linear low-sulfur adjustment A_s .

$$A_s = 1.0 - \beta_s (S_{base} - x_s) \quad \text{Equation 3-20}$$

The Tier 2 Low Sulfur coefficients (β_s) were developed by linearly interpolating between the emission levels at 28 to 5 ppm, corresponding to the reductions in emissions shown in Table 3-24, relative to a base sulfur level of 30 ppm. The sulfur coefficient simply represents the slope of the interpolated line between 28 and 5 ppm fuel sulfur levels on emissions. Values of the coefficients vary among pollutants and processes (i.e., start vs. running, as applicable). The term S_{base} represents a “base” sulfur level of 30 ppm for vehicles in model years after 2000. Finally, x_s represents the sulfur level for the fuel being modeled in a MOVES run.

The linearity of sulfur impacts on emissions is supported by past studies with multiple fuel sulfur levels all of which compare gasoline with differing sulfur levels below 100 ppm (e.g., CRC E-60 and 2001 AAM/AIAM programs). The emission reductions from FTP bag 2 and FTP bag1-bag3 were used to calculate the sulfur coefficients for running exhaust and start exhaust, respectively. The percent reduction estimates from all Tier 2-certified vehicles from the in-use sulfur test program were used to develop the sulfur coefficients for passenger cars, passenger trucks, and light commercial trucks. For heavier gasoline vehicles, a separate mixed model analyses were performed on Tier 2 Bin 8 vehicles from the in-use sulfur test program, as described earlier, and the resulting estimates of percent reduction (Table 3-24) were used to develop the coefficients for heavy-duty gasoline vehicles, assuming that the catalyst response of heavier gasoline trucks to fuel sulfur level is closer to Tier 2 Bin 8 vehicles than to lower standard levels. Due to a lack of data, we assumed no impact of sulfur on emissions for 2001-and-later motorcycles. **Table 3-28** shows the specific values of the sulfur coefficients used in T2LowSulf model by pollutant, process, and vehicle type.

The sulfur base (S_{base}) in the T2LowSulf model varies as a function of model year group. For model year group 2001-2016, the sulfur base is unchanged at 30 ppm. However, for model year group 2017-2050, since the Tier 3 emission rates in MOVES assume that Tier 3 vehicles run on 10 ppm sulfur, the sulfur base is set at 10 ppm to prevent double-counting of the impacts of low levels of sulfur in fuels for Tier 3 vehicles. x_s represents the actual in-use sulfur levels in the region being modeled.

Table 3-28. Interpolated Coefficients by Vehicle Type, Process and Pollutant, applied for sulfur levels < 30 ppm

Vehicle Type	THC		CO		NO _x		PM	
	Starts	Running	Starts	Running	Starts	Running	Starts	Running
Motorcycle	0	0	0	0	0	0	0	0
Passenger Car, Passenger Truck & Light Commercial Truck	0.002568	0.018126	0	0	0	0.021582	0	0
All other Vehicle Types	0	0.015488	0	0.009436	0	0.027266	0	0

Equation 3-20 has been applied using the coefficients in **Table 3-28** in the database table that stores the fuel effect equations in the MOVES database (“*generalFuelRatioExpression*”). This table consolidates the two sulfur models (M6Sulf and T2LowSulf) for MYG 2001-2016 and 2017-2050, and the other fuel-effect models (i.e., EPAAct model, discussed later), and allows the MOVES model to compute the fuel effects based on the fuel properties of any fuel contained in the “*fuelSupply*” and “*fuelFormulation*” database tables. A detailed description of the “*generalFuelRatioExpression*” table is shown in Section 6.5 (page 87).

3.4 Results: Sulfur Effects in MOVES2014

The trends in emissions in relation to fuel sulfur levels are shown in Figure 3-8 through Figure 3-11 for the 2017+, 2001-2016, 1996 and 1988 model years, respectively, for passenger cars, passenger and light commercial trucks. The effects are ‘net fuel effects’ for running-exhaust emissions from the MOVES model. They were produced by compiling results from eight separate MOVES runs using a constant fuel formulation and varying the fuel sulfur level from 4 ppm sulfur to 500 ppm sulfur. The 1988 model year represents the fuel effects on Tier 0 vehicles, and the 1996 model year represents the Tier1 and LEV standards, applying log-log and log-linear relationships within the M6Sulf model, as previously described; the 2001-2016 model year represent Tier 2 vehicles, and the 2017+ model years represent Tier 3 vehicles.

The fuel effects are normalized to 90 ppm sulfur for model years 1988 to 1996, to 30 ppm sulfur for model years 2001 to 2016, and to 10 ppm sulfur for model years 2017 and later. In this context, ‘normalization’ means the correction factor is set to 1.0 at the specified level. For these examples, the other fuel parameters were set at Base-Fuel levels (RVP at 6.9 psi, 0% Ethanol volume, 26.1% aromatic content, 5.6% olefin content, 1.0% benzene content, T50 at 218°F and T90 at 329°F).

It is worth noting that, in contrast to NO_x and THC, the fuel sulfur adjustment for running CO for MY 2001 and later is equal to 1.0 for all fuel sulfur levels less than 30 ppm (Figure 3-8 and Figure 3-9). This pattern is applied because the sulfur coefficient for running CO (**Table 3-28**) is zero in the T2Sulfur model for passenger cars, passenger and light commercial trucks.

Figure 3-8. Relative Fuel Sulfur Effects for Running-Exhaust Emissions for MY 2017 and later, normalized to a sulfur level of 10 ppm.

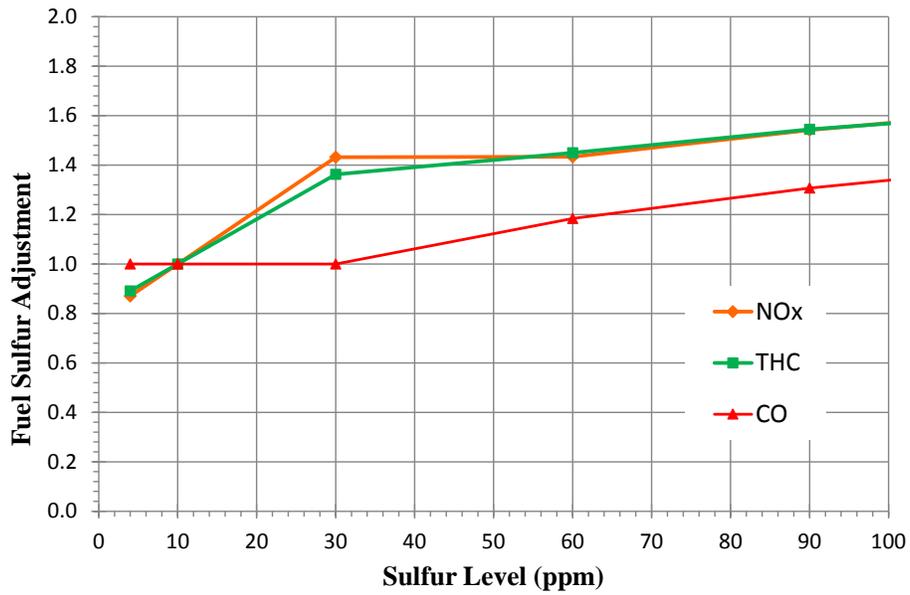


Figure 3-9. Relative Fuel Sulfur Effect for Running Exhaust Emissions for MYs 2001 to 2016, normalized to a sulfur level of 30 ppm.

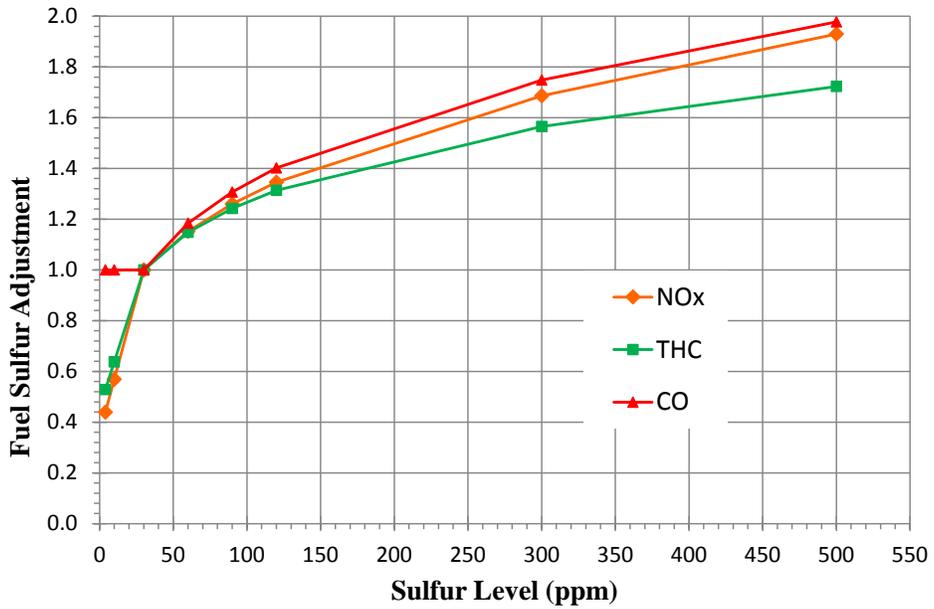


Figure 3-10. Relative Fuel Sulfur Effect for Running Exhaust Emissions for MY 1996, normalized to a sulfur level of 90 ppm.

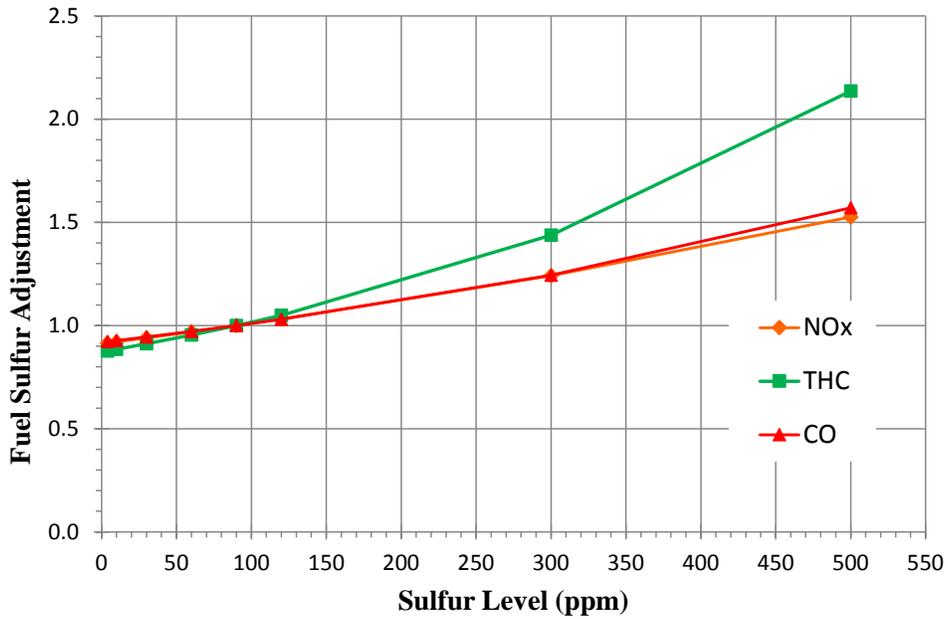
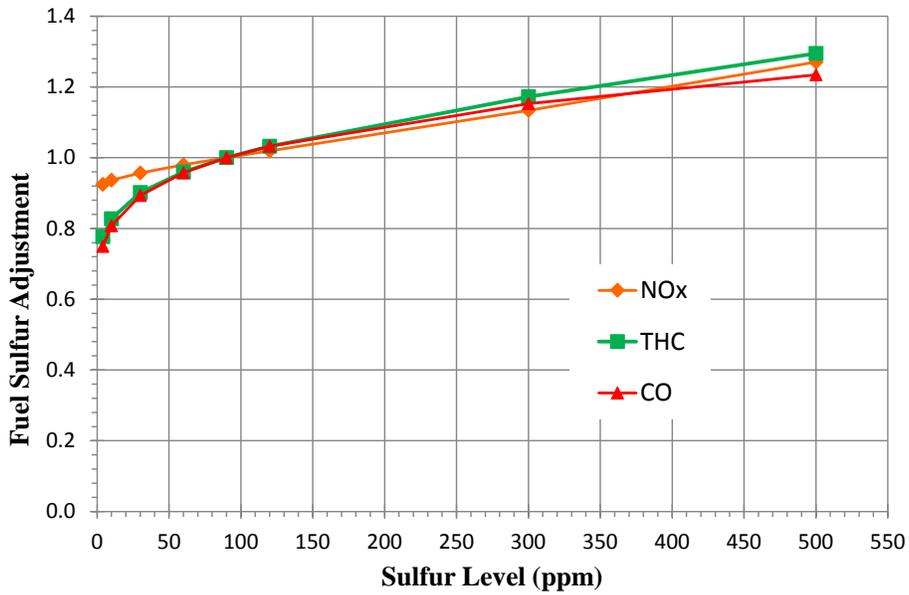


Figure 3-11. Relative Fuel Sulfur Effect for Running Exhaust Emissions for MY 1988, normalized to a sulfur level of 90 ppm.



4 Use of the Complex Model (for CO Emissions)

For carbon monoxide, fuel adjustments were estimated through application of equations developed for the Complex Model for Reformulated Gasoline.³⁸ The “Complex Model” is so called because it was designed to model the “complex” behavior of selected pollutants in relation to changes in a set of selected fuel properties. By contrast, a “simple model” is a uniform ratio or fraction that does not vary in response to fuel properties.

The Complex Model equations are applied to running, start and extended-idle emissions for gasoline-fueled vehicles for all 2000 and earlier model years. For 1974 and earlier model years, 1975 weightings are used. In addition, while MOBILE6.2 relied on very limited data from heavy-duty gasoline vehicles, MOVES applies Complex Model equations to both light-duty and heavy-duty gasoline vehicles. This step was taken because the very limited data specific to heavy-duty gasoline vehicles are not adequate to account for effects of fuel properties.

4.1 Overview of the Complex Model

The underlying dataset included measurements collected on sample of vehicles manufactured in MY1990 or earlier, and reflecting “Tier 0” standards, over a variety of gasoline formulations.

The complex model is composed of sets of models for each pollutant. The models are statistical models fit to sets of emissions measurements on a set of fuels with widely varying properties. For CO, the model includes linear terms for six properties, quadratic terms for four properties, and one interaction term, as shown in Table 4-1. Note that in the database table *ComplexModelParameters*, model terms are represented by a cmpID, which is defined in the translation table *ComplexModelParameterName*. For convenience, relevant values of cmpID are also translated in Table 4-4 below.

For CO, 10 models were fit, with each representing a specific combination of fuel-delivery, catalyst, air injection and emissions-control technology. The technology groups are described in Table 4-2. As an aggregate, these sets of models are referred to as the “unconsolidated complex model.”

In fitting the complex models, the measurements for all fuel properties were “centered,” meaning that the mean of all measurements for the property was subtracted from each individual measurement. This step aids in scaling the dataset so that each fuel property is centered on a mean of 0.0. Thus, if $\ln Y$ is the natural logarithm of a emissions, the model is fit as shown in Equation 4-1, using terms for oxygenate (wt.%), aromatics (vol.%) and RVP (psi) as examples for linear terms, and E300×OLE as an example of a 2nd-order interaction term. Note that squared (quadratic) terms are centered similarly to the interaction term.

$$\ln Y = \beta_0 + \beta_{\text{oxy}} (x_{\text{oxy},i} - \bar{x}_{\text{oxy}}) + \beta_{\text{arom}} (x_{\text{arom},i} - \bar{x}_{\text{arom}}) + \dots + \beta_{\text{RVP}} (x_{\text{RVP},i} - \bar{x}_{\text{RVP}}) + \dots \\ \dots + \beta_{\text{E300OLE}} (x_{\text{E300},i} - \bar{x}_{\text{E300}})(x_{\text{OLE},i} - \bar{x}_{\text{OLE}}) \quad \text{Equation 4-1}$$

The mean values used for centering all individual fuel–property values are presented in Table 4-3. The set of coefficients (β values in Equation 4-1) for the CO models by technology group, are presented in Table 4-4 and Table 4-5, which contain linear and 2nd-order terms, respectively. Note that in the database table *ComplexModelParameters*, the values are stored in two fields, *coeff1* and *coeff2*. The values in the tables below are the sums of these two fields. In the model fitting, *coeff1* represents a coefficient for all 11 groups as an aggregate, and *coeff2* represents an adjustment to the aggregate term to represent a difference between the main model (for all groups) and the model specific to a group.

It should be noted that the sulfur effects terms in the original complex model were not included when the model was adapted for inclusion in MOVES. Rather, the effects of fuel sulfur are estimated independently, due to the propensity of sulfur to reduce catalyst efficiency and confound the effects of other fuel properties.

Table 4-1. Definition and Description of Terms included in the Complex Model for CO.

cmpID	cmpName	Description
1	OXYGEN	Oxygenate
6	AROMATIC	Aromatics Content
7	OLEFINS	Olefin content
3	RVP	Reid Vapor Pressure
4	E200	Percent Fuel evaporated at 200 °F
5	E300	Percent Fuel evaporated at 300 °F
15	OLESQR	Olefin × Olefin
11	RVPSQR	RVP × RVP
12	E200SQR	E200 × E200
13	E300SQR	E300 × E300
22	E300OLE	E300 × Olefins

Table 4-2. Technology Groups included in the Complex Model.

Technology Group	Fuel System ¹	Catalyst ²	Air Injection	Exhaust-gas Recirculation
1	PFI	3-Way	No	Yes
2	PFI	3-Way	No	No
3	TBI	3-Way	No	Yes
4	PFI	3-Way + Oxy	Yes	Yes
5	PFI	3-Way	Yes	Yes
6	TBI	3-Way	Yes	Yes
7	TBI	3-Way + Oxy	Yes	Yes
8	TBI	3-Way	No	No
9	carburetor	3-Way + Oxy	Yes	Yes
10 (“High Emitters”)	ALL	ALL	ALL	ALL

¹ Fuel System: PFI = port fuel Injection, TBI = throttle body injection.
² Catalyst type: “3-way” = three-way catalyst, “Oxy” = oxidation catalyst.

Table 4-3. Mean Fuel-Property Values used for centering Terms in the Complex Model for CO.¹

Property	fuelParameterID	Units	Base Value ²	Mean Value
Aromatics	6	Vol. %	32	28.26110
Olefins	7	Vol. %	9.2	7.318716
Oxygenate	1	Wt.%	0	1.774834
RVP	3	psi	8.7	8.611478
E200	4	%	41	46.72577
E300	5	%	83	85.89620

¹ Stored in database table *meanFuelParameters* where polprocessid = 201 or 202.
² Value for base fuel.

Table 4-4. Complex Model Coefficients for Linear Effects, for Carbon Monoxide, by Technology Group.

Technology Group	Fuel Property					
	Oxygen	Aromatics	Olefins	RVP	E200	E300
1	-0.032584	0.007795	0.000507	0.043314	-0.002335	0.002372
2	-0.019006	0.00547	0.000507	0.003448	-0.002335	0.002372
3	-0.019006	0.00547	0.000507	0.003448	-0.002335	-0.009238
4	-0.095314	0.00547	0.000507	0.003448	0.005751	0.002372
5	-0.019006	0.000365	0.000507	0.003448	-0.002335	0.002372
6	-0.019006	0.00547	0.000507	0.003448	-0.002335	-0.002211
7	-0.019006	0.00547	0.000507	0.003448	-0.002335	0.002372
8	-0.019006	0.00547	0.000507	0.003448	-0.002335	0.002372
9	-0.019006	0.00547	0.000507	0.003448	-0.002335	0.002372
10	-0.019006	0.00547	0.000507	0.003448	-0.002335	0.002372
11	-0.032584	0.007795	0.000507	0.043314	-0.002335	0.002372

Table 4-5. Complex Model Coefficients for 2nd-Order Effects, for Carbon Monoxide, by Technology Group.

Technology Group	Fuel Property				
	OLESQR	RVFSQR	E200SQR	E300SQR	E300OLE
1	0.000291	0.017288	0.000078	0.000515	0.000362
2	-0.000104	0.007093	0.000078	0.000515	0.000362
3	-0.000104	0.007093	0.000217	0.000515	-0.000511
4	0.000605	0.007093	0.000078	0.000515	0.000362
5	-0.000104	0.007093	0.000078	0.000515	0.000362
6	-0.000104	0.007093	0.000078	0.000515	-0.000244
7	-0.000104	0.007093	0.000078	0.000515	0.000362
8	-0.000104	0.007093	0.000078	0.000515	0.000362
9	-0.000104	0.007093	0.000078	0.000515	0.000362
10	-0.000104	0.007093	0.000078	0.000515	0.000362
11	0.000291	0.017288	0.000078	0.000515	0.000362

4.2 Application of the Complex Model

For each compound, the model equations are evaluated for a “base” and a “target” fuel (See Section 1). The base fuel represents a fuel assumed to be that reflected in the base emission rates and which serves as a basis for fuel adjustments. The target fuel is represented by a specific set of properties and which represents a fuel “in-use” in the geographic area(s) and season(s) being modeled.

Initially, an adjustment for the difference in emissions of the compound modeled on the target fuel relative to the base fuel is calculated. If the model, as shown above, can be conveniently expressed, using matrix notation, as $\mathbf{X}\beta_{\text{target}}$ and $\mathbf{X}\beta_{\text{base}}$ for estimates on the target and base fuels, then the fractional difference in emissions is given by

$$f_{\text{adj}} = \frac{\exp(\mathbf{X}\beta_{\text{target}})}{\exp(\mathbf{X}\beta_{\text{base}})} - 1.0 \quad \text{Equation 4-2}$$

The expression in Equation 4-2 is evaluated for target and base fuels for each of the ten technology groups. A mean value of the adjustment is then calculated for each model year from 2000 to 1970, as a weighted average of the fraction of sales in each group in each model year, for the groups, as shown in Equation 4-3. The weights are shown in Table 4-6 and represent the sales fractions for the ten vehicle technologies at each age.

Note that the use of varying weights in applying the complex model in MOVES differs from the original application in which the weights were invariant. The application of Equation 4-3 to each of the 30 model years gives a set of 30 adjustments, with each applied to its respective model year.

$$f_{\text{adj,mean}} = \sum_{\text{Group}=1}^{10} w_{\text{Group}} f_{\text{adj,Group}} \quad ; \quad \sum_{\text{Group}=1}^{10} w_{\text{Group}} = 1.0 \quad \text{Equation 4-3}$$

The mean adjustments calculated in Equation 4-3 are then applied to estimate emissions of CO on the target fuel (E_{relative}), representing the effect on the emissions of CO due to the changes in fuel properties between the target and base fuels (Equation 4-4). If the target and base fuels were identical, the values of $f_{\text{adj,mean}}$ would be 0.0.

$$E_{\text{relative}} = E_{\text{base}} (1 + f_{\text{adj,mean}}) \quad \text{Equation 4-4}$$

Note that the weights used in MOVES differ from those originally used in the Complex model for purposes of fuel certification. They now vary by age to reflect the changing importance of technology groups (weights in the original do not vary). There is now less emphasis on so called “High emitters”. The original Complex model gave a 55 percent weighting to high emitters (i.e., fuel model = 10). Group 10 now receives a weighting ranging from 0.01 percent at age zero to 32.8 percent at age 30.

The final adjustment for non-sulfur properties, calculated as described in this section, is then multiplied by the adjustment for sulfur, calculated as described above in Section 3.2 (page 9). Note that the fuel adjustment for CO is applied only to vehicles in model years 1975 to 2003. For model years 1974 and earlier, the adjustment is reset to 1.0, i.e., no adjustment is applied.

Table 4-6. Weights Applied to Complex Model coefficients for Technology Groups, by Age (Vehicle Age 0 represents model year 2000).^a

Age	Technology Group									
	1	2	3	4	5	6	7	8	9	10
0	0.2360	0.2829	0.1806	0.1814	0.0290	0.0042	0.0556	0.0	0.0203	0.0100
1	0.2339	0.2803	0.1789	0.1797	0.0287	0.0042	0.0551	0.0	0.0201	0.0190
2	0.2315	0.2774	0.1771	0.1779	0.0284	0.0041	0.0546	0.0	0.0199	0.0290
3	0.2272	0.2723	0.1738	0.1746	0.0279	0.0041	0.0536	0.0	0.0196	0.0470
4	0.2229	0.2672	0.1706	0.1713	0.0274	0.0040	0.0525	0.0	0.0192	0.0650
5	0.2189	0.2623	0.1675	0.1682	0.0269	0.0039	0.0516	0.0	0.0188	0.0820
6	0.2148	0.2574	0.1644	0.1651	0.0264	0.0038	0.0506	0.0	0.0185	0.0990
7	0.2110	0.2529	0.1614	0.1621	0.0259	0.0038	0.0497	0.0	0.0182	0.1150
8	0.2072	0.2483	0.1585	0.1592	0.0254	0.0037	0.0488	0.0	0.0178	0.1310
9	0.2036	0.2440	0.1558	0.1565	0.0250	0.0036	0.0480	0.0	0.0175	0.1460
10	0.2000	0.2397	0.1530	0.1537	0.0246	0.0036	0.0471	0.0	0.0172	0.1610
11	0.1967	0.2357	0.1505	0.1512	0.0241	0.0035	0.0464	0.0	0.0169	0.1750
12	0.1934	0.2317	0.1479	0.1486	0.0237	0.0035	0.0456	0.0	0.0166	0.1890
13	0.1903	0.2280	0.1456	0.1462	0.0234	0.0034	0.0448	0.0	0.0164	0.2020
14	0.1872	0.2243	0.1432	0.1438	0.0230	0.0033	0.0441	0.0	0.0161	0.2150
15	0.1843	0.2209	0.1410	0.1416	0.0226	0.0033	0.0434	0.0	0.0159	0.2270
16	0.1814	0.2174	0.1388	0.1394	0.0223	0.0032	0.0428	0.0	0.0156	0.2390
17	0.1786	0.2140	0.1366	0.1372	0.0219	0.0032	0.0421	0.0	0.0154	0.2510
18	0.1760	0.2109	0.1346	0.1352	0.0216	0.0031	0.0415	0.0	0.0151	0.2620
19	0.1736	0.2080	0.1328	0.1334	0.0213	0.0031	0.0409	0.0	0.0149	0.2720
20	0.1712	0.2052	0.1310	0.1315	0.0210	0.0031	0.0403	0.0	0.0147	0.2820
21	0.1688	0.2023	0.1291	0.1297	0.0207	0.0030	0.0398	0.0	0.0145	0.2920
22	0.1664	0.1994	0.1273	0.1279	0.0204	0.0030	0.0392	0.0	0.0143	0.3020
23	0.1643	0.1969	0.1257	0.1262	0.0202	0.0029	0.0387	0.0	0.0141	0.3110
24	0.1624	0.1946	0.1242	0.1248	0.0199	0.0029	0.0383	0.0	0.0140	0.3190
25	0.1602	0.1920	0.1226	0.1231	0.0197	0.0029	0.0378	0.0	0.0138	0.3280
26	0.1602	0.1920	0.1226	0.1231	0.0197	0.0029	0.0378	0.0	0.0138	0.3280
27	0.1602	0.1920	0.1226	0.1231	0.0197	0.0029	0.0378	0.0	0.0138	0.3280
28	0.1602	0.1920	0.1226	0.1231	0.0197	0.0029	0.0378	0.0	0.0138	0.3280
29	0.1602	0.1920	0.1226	0.1231	0.0197	0.0029	0.0378	0.0	0.0138	0.3280
30	0.1602	0.1920	0.1226	0.1231	0.0197	0.0029	0.0378	0.0	0.0138	0.3280

^a Note that in the MOVES database, these weights are stored in the table FuelModelWtFactor.

5 Use of the EPA Predictive Model (HC and NO_x Emissions)

For hydrocarbon and NO_x emissions, “complex” fuel adjustments are estimated not through application of the Complex Model, but rather through application of equations developed for the “EPA Predictive Model” (EPM). The Predictive Model was applied for these two pollutants because it represents more recent work than the Complex Model, although modeling for CO was not included in the effort.

The EPM is composed of sets of statistical models developed during evaluation of a petition by the State of California for a waiver of the Federal oxygenate requirement for reformulated gasoline.³⁹ The EPM predicts changes in NO_x and HC emissions from changes in fuel properties, and was initially developed in the course of EPA’s evaluation of the “CARB Phase-3 Predictive Model,” developed to “*allow evaluation of gasoline specifications, ... , as alternatives to the flat and average property limits on gasoline specifications in California’s regulations.*” After reviewing technical analyses submitted by the State of California, EPA elected to pursue an independent modeling effort, in large part due to “*a substantial disparity between the NO_x-oxygen relationship that emerges from the Phase 3 Model and from the other two major modeling efforts – the EPA Complex Model and the CARB Phase 2 model.*”

5.1 Data Used in Developing the EPA Predictive Model

In developing the EPM, EPA used the same dataset used by California, with some additions, modifications and exclusions. Specifically, EPA confined its efforts to sets of data for vehicles manufactured in model years 1986 to 1993, designated as “Tech 4” vehicles. EPA elected not to revisit models for vehicles manufactured prior to 1986 (“Tech 3”) or in 1996 and later (“Tech 5”), which were included in the CARB models. As the analysis concerned application of regulations in California, only vehicles certified to California standards were included. Additionally, observations with “extreme” fuel-property values or measured at ambient temperatures outside the range of 68-95 °F were excluded. Finally, observations missing values for any of the fuel properties under study were removed.

5.2 Analytic Approaches

As in the Complex Model, models were fit to the natural logarithm of emissions results, applied as a normalizing and variance-stabilizing transformation.

The models were fit as “mixed” models, with fuel properties as “fixed” and vehicles as “random” effects. In a departure from the approach used by CARB, EPA chose to include separate terms for “high emitters,” as in the Complex model, whereas CARB had not distinguished “high emitters” in its Phase-3 model.

Model fitting was performed in a series of steps. In the first step, all linear effects were included in an initial model, and second-order quadratic and interaction terms were selected for inclusion through a forward stepwise process. During stepwise fitting, 2nd-order terms with individual *p*-values increasing to levels exceeding a 5.0% confidence level upon the addition of subsequent terms were removed. Again, all linear terms were retained at this stage, regardless of their individual confidence levels.

Models developed in the first step were further evaluated using two information criteria (AIC and BIC). At the culmination of model fitting, single models were not selected for each pollutant. Rather sets of models were retained for application, with overall results to be obtained by averaging the results for individual models.

The MOVES database contains sets of coefficients for NO_x and THC. The models include linear terms for six properties, with additional quadratic or interaction terms, as shown in Table 5-1. Note that in the database table *ComplexModelParameters*, model terms are represented by a cmpID, which is defined in the translation table *ComplexModelParameterName*. For convenience, relevant values of cmpID are also translated in Table 5-1.

Table 5-1. Definition and Description of Terms included in the Predictive Model for NO_x and THC.

cmpID	cmpName	Description
52	Intercept	Intercept term
1	OXYGEN	Oxygenate
6	AROMATIC	Aromatics Content
7	OLEFINS	Olefin content
3	RVP	Reid Vapor Pressure
54	T50	T50 (°F)
55	T90	T90 (°F)
57	T50SQR	Quadratic term for T50
56	T90SQR	Quadratic term for T90
63	OXYT50	Oxygenate × T50 interaction
58	OXYT90	Oxygenate × T90 interaction
60	AROT90	Aromatics × T90 interaction
61	T50HI	Distinct T50 slope for “high emitters”
53	HI	Distinct intercept for “high emitters”

5.2.1 Standardization of Fuel Properties

In fitting the predictive models, the measurements for all fuel properties were “centered,” meaning that the mean of all measurements for the property was subtracted from each individual measurement. The centered measurement, representing the distance between the measurement and its mean (positive or negative) was then “scaled” by dividing it by the standard deviation of all measurements. These steps, known as “standardization,” aided in scaling the dataset so that each fuel property is centered on a mean of 0.0 and expressed in units of its own standard deviation, which places the various fuel properties into a common “space” for purposes of analysis. The result, designated as “Z” was calculated as shown in Equation 5-1, using the aromatics term as an example. Means and standard deviations for the properties used in standardization are shown in Table 5-2.

$$Z_{\text{ARO}} = \frac{(x_{\text{ARO},i} - \bar{x}_{\text{ARO}})}{s_{\text{ARO}}}$$

Equation 5-1

The standardization for a 2nd-order term, i.e., a quadratic or interaction term is calculated by multiplying the individual standardized terms, as shown in Equation 5-2 for a squared term (T50×T50), and in Equation 5-3 for an interaction term (ARO×T90).

$$Z_{T50SQR, i} = Z_{T50,i} Z_{T50,i} = \left(\frac{(x_{T50,i} - \bar{x}_{T50})}{s_{T50}} \right)^2 \quad \text{Equation 5-2}$$

$$Z_{AROT90,i} = Z_{ARO,i} Z_{T90,i} = \left(\frac{(x_{ARO,i} - \bar{x}_{ARO})}{s_{ARO}} \right) \left(\frac{(x_{T90,i} - \bar{x}_{T90})}{s_{T90}} \right) \quad \text{Equation 5-3}$$

Table 5-2. Fuel-Property Values used to Standardize Terms in the Predictive Model.¹

Property	fuelParameterID	Units	Base Value ²	Mean Value	Std. Dev.
Aromatics	6	Vol. %	26.1	28.0828	7.38317
Olefins	7	Vol. %	5.6	6.97437	4.93287
Oxygenate	1	Wt.%	0	1.34763	1.25188
RVP	3	psi	6.9	8.44534	0.780184
T50	9	°F	218	206.816	17.9063
T90	10	°F	329	312.126	22.0993

¹ Stored in database table *meanFuelParameters* where *polprocessid* = 101,102, 301 or 302.
² Value for base fuel.

Thus, if lnY is the natural logarithm of a species such as NO_x, the model is fit as shown in Equation 5-4, using terms for oxygenate (wt.%), aromatics (vol.%) and RVP (psi) as examples for linear terms, and T50SQR and AROT90 terms as examples of 2nd-order quadratic and interaction terms, respectively.

$$\ln Y = \beta_0 + \beta_{OXY} Z_{OXY} + \beta_{ARO} Z_{ARO} + \dots + \beta_{RVP} Z_{RVP} + \dots \quad \text{Equation 5-4}$$

$$\dots + \beta_{T50SQR} Z_{T50SQR} + \beta_{AROT90} Z_{AROT90} + \dots$$

The sets of coefficients (β values in the equation) for the NO_x models are presented in Table 5-3 and Table 5-4, which contain linear and 2nd-order terms, respectively. Corresponding terms for the HC models are presented in Table 5-5 and Table 5-6. The tables include six candidate model fits for NO_x and three for HC. When the models are applied, an unweighted average of results for

all candidate models is calculated and used to calculate fuel effects. Note that in the database table *ComplexModelParameters*, the values are stored in a single field *coeff1*.

It should be noted that the sulfur effects terms in the original Predictive Model were not included when the model was adapted for inclusion in MOVES; rather, the effects of fuel sulfur are estimated independently, due to the propensity of sulfur to reduce catalyst efficiency and confound the effects of other fuel properties. The effects of fuel sulfur are discussed in Chapter 3.

Table 5-3. NO_x: Predictive Model Coefficients for Linear Effects for Six Candidate Models.

Candidate Model	Fuel Property							
	Intercept ¹	H ₂	Oxygen	Aromatics	Olefins	RVP	T50	T90
302 (Step-2)	-0.6603	0.396	0.0124	0.01587	0.01988	0.009093	-0.00245	0.00719
303 (3)	-0.6606	0.3963	0.01728	0.01431	0.01949	0.01172	0.000084	0.007879
304 (Step-3)	-0.6656	0.3965	0.01333	0.01524	0.0194	0.009694	0.001804	0.005543
305 (5)	-0.6651	0.396	0.01371	0.01407	0.01966	0.007673	0.001173	0.006239
306 (6)	-0.6624	0.3961	0.01351	0.01501	0.0199	0.00839	0.000312	0.006213
307 (7)	-0.6737	0.3969	0.008245	0.01209	0.01969	0.006188	-0.00475	0.007587

¹ The original values from model fitting are presented in the table; in the MOVES application, this term is reset to 1.0.

Table 5-4. NO_x: Predictive Model Coefficients for 2nd-Order Effects for Six Candidate Models.

Candidate Model	Fuel Property				
	OXSQR	T50SQR	OXYARO	OXYT50	OXYT90
302 (Step-2)					
303 (3)					-0.0051
304 (Step-3)		0.006974			
305 (5)				-0.0083	
306 (6)			-0.00547		
307 (7)	0.0112				

Table 5-5. HC: Predictive Model Coefficients for Linear Effects for Three Candidate Models.

Candidate Model	Fuel Property							
	Intercept ¹	HI ¹	Oxygen	Aromatics	Olefins	RVP	T50	T90
107	-1.5957	1.6909	-0.01329	0.008729	-0.01426	0.008474	0.06125	0.02084
108	-1.598	1.6935	-0.01378	0.008465	-0.0143	0.008971	0.06499	0.02104
112	-1.6012	1.7091	-0.01391	0.008759	-0.01457	0.007973	0.06046	0.02133

¹ The original values from model fitting are presented in the table; in the MOVES application, this term is reset to 1.0.

Table 5-6. HC: Predictive Model Coefficients for 2nd-Order Effects for Three Candidate Models.

Candidate Model	Fuel Property					
	OXY5QR	T505QR	T905QR	OXYT90	AROT90	T50HI
107	0.01256	0.02494	0.01617	0.01589	0.006908	
108	0.01353	0.02477	0.01604	0.01576	0.007013	-0.02609
112	0.01288	0.02469	0.01633	0.01552	0.006814	

5.3 Application in MOVES

The application of the EPM in MOVES differs from its regulatory application in certain respects, as described below. The Predictive Model equations are applied to running, start and extended idle emissions for gasoline-fueled vehicles over MY range 1960-2000. In addition, while MOBILE6.2 relied on very limited data from heavy-duty gasoline vehicles, MOVES applies Predictive Model equations to both light-duty and heavy-duty gasoline vehicles. This step was taken because the very limited data specific to heavy-duty gasoline vehicles are not adequate to account for effects of fuel properties.

For each compound, the model equations as shown in the tables above, are evaluated for “base” and “target” fuels (as defined in Chapter 1 above (page 3)). The base fuel represents a fuel assumed to be reflected in the base emission rates and which serves as a basis for fuel adjustments. The target fuel is represented by a specific set of properties and which represents a fuel “in-use” in the geographic area(s) and season(s) being modeled.

Initially, an adjustment for the difference in emissions of the compound modeled on the target fuel relative to the base fuel is calculated. If the model, as shown in Equation 5-4, can be conveniently expressed, using matrix notation, as $X\beta_{\text{target}}$ and $X\beta_{\text{base}}$ for estimates on the target and base fuels, then the ratio difference in emissions is given by Equation 5-5.

$$f_{\text{adj}} = \frac{\exp(\mathbf{X}\boldsymbol{\beta}_{\text{target}})}{\exp(\mathbf{X}\boldsymbol{\beta}_{\text{base}})} \quad \text{Equation 5-5}$$

The adjustment for the non-sulfur properties developed as described in this chapter is multiplied by the adjustment for sulfur, which is derived as described above in Section 3.2 (page 9). Note that the fuel adjustments for HC and NO_x are applied only to vehicles in model years 1975 to 2003. For model years 1974 and earlier, the adjustment is reset to 1.0, i.e., no adjustment is applied.

6 Gasoline Fuel Effects for Vehicles certified to Tier-2 Standards (EPA Act Models: HC, CO, NO_x, PM)

6.1 Introduction: the EPA Act Project

An important function of mobile source air pollution inventory models, including MOBILE6 and MOVES, is to account for the effects of different fuel properties on exhaust emissions. For this purpose, MOBILE6 relied on previously existing fuel effect models, known as the “EPA Predictive Model” and the “Complex Model”. These models were developed using data collected on 1990s-technology vehicles, with emissions levels an order of magnitude higher than those for currently manufactured vehicles compliant with Federal Tier-2 or equivalent LEV-II standards. These models are still in use in MOVES to estimate fuel effects for vehicles manufactured prior to model year 2001, as described in the previous two chapters. For example, equations from the Predictive Model are used to calculate fuel effects for total hydrocarbons and oxides of nitrogen, and equations from the Complex Model are used to estimate fuel effects for carbon monoxide and air toxics, such as benzene and the aldehydes.⁴⁰ More recently, the applicability of older models to vehicles employing more recent engine and emission control technologies has been questioned. Since the initiation of the MOVES project, it has become clear that an updated fuel-effects model representing Tier-2 certified vehicles would be needed. In addition, Congress provided for the development of such a model in the 2005 Energy Policy Act (EPA Act).

To meet this goal, EPA entered a partnership with the Department of Energy (DOE) and the Coordinating Research Council (CRC) to undertake the largest fuels research program conducted since the Auto/Oil program in the early 1990’s, aimed specifically at understanding the effects of fuel property changes on exhaust emissions on recently manufactured Tier 2 vehicles. The resulting research program was dubbed the “EPA Act/V2/E-89” program (or “EPA Act”), with the three components of the label denoting the designation given to the study by the EPA, DOE and CRC, respectively.

The program was conducted in three phases. Phases 1 and 2 were pilot efforts involving measurements on 19 light-duty cars and trucks on three fuels, at two temperatures. These preliminary efforts laid the groundwork for design of a full-scale research program, designated as Phase 3.

Initiated in March 2009, the Phase 3 program involved measurement of exhaust emissions from fifteen high-sales-volume Tier-2 certified vehicles. The vehicles were selected so as to represent the latest technologies on the market at the time the program was launched (2008). The vehicles were to reflect a majority of sales for model year 2008. In addition, the vehicles were to conform primarily to Tier-2 Bin-5 exhaust standards, and to reflect a variety of emission-control technologies, as realized through the selection of a range of vehicles sizes and manufacturers. The vehicle sample is summarized in Table 6-1.

Table 6-1. Test Vehicles for the Phase-3 EPAAct Program (all vehicles in MY2008).

Make	Brand	Model	Engine Size	Tier 2 Bin	LEVII Std	Odometer
GM	Chevrolet	Cobalt	2.2L I4	5	NA	4,841
GM	Chevrolet	Impala FFV	3.5L V6	5	L2	5,048
GM	Saturn	Outlook	3.6L V6	5	L2	5,212
GM	Chevrolet	Silverado FFV	5.3L V8	5	NA	5,347
Toyota	Toyota	Corolla	1.8L I4	5	U2	5,019
Toyota	Toyota	Camry	2.4L I4	5	U2	4,974
Toyota	Toyota	Sienna	3.5L V6	5	U2	4,997
Ford	Ford	Focus	2.0L I4	4	U2	5,150
Ford	Ford	Explorer	4.0L V6	4	NA	6,799
Ford	Ford	F150 FFV	5.4L V8	8	NA	5,523
Chrysler	Dodge	Caliber	2.4L I4	5	NA	4,959
Chrysler	Jeep	Liberty	3.7L V6	5	NA	4,785
Honda	Honda	Civic	1.8L I4	5	U2	4,765
Honda	Honda	Odyssey	3.5L V6	5	U2	4,850
Nissan	Nissan	Altima	2.5L I4	5	L2	5,211

The study used a set of twenty-seven test fuels spanning wide ranges of five fuel properties (ethanol, aromatics, vapor pressure, and two distillation parameters: T50 and T90). The numbers of test points and values of each property are shown in Table 6-2. The properties of the test fuels were not assigned to represent in-use fuels, but rather to allow development of statistical models that would enable estimation of relative differences in emissions across the ranges of fuel properties expected in commercially available summer fuels in the U.S. (5th to 95th percentiles for each property).

Table 6-2. Levels assigned to Experimental Factors (Fuel parameters) for the Phase-3 EPAAct program.

Factor	No. Levels	Levels		
		Low	Middle	High
Ethanol (vol.%)	4	0	10, 15	20
Aromatics (vol.%)	2	15		35
RVP (psi)	2	7		10
T50 (°F)	5	150	165, 190, 220	240
T90 (°F)	3	300		340

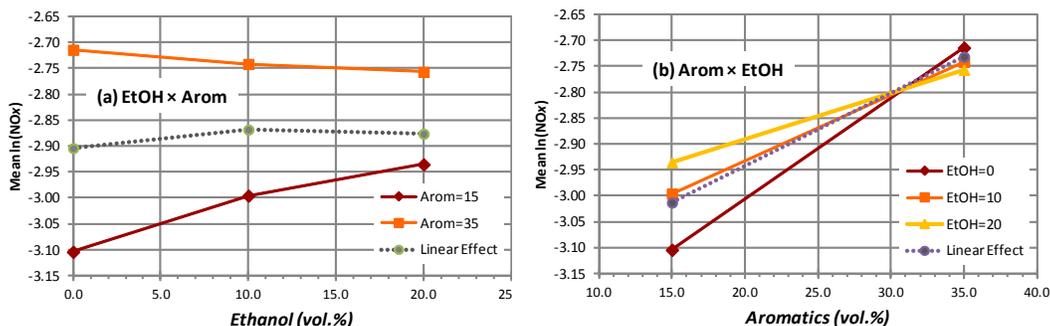
The experimental design embodied in the fuel set is the product of an iterative process involving balancing among research goals, fuel-blending feasibility and experimental design. As fuel properties tend to be moderately to strongly correlated, and as the goal was to enable analysis of fuel effects as though the properties were independent (uncorrelated), it was necessary to address these issues in design and analysis. Accordingly, the fuel set was designed using a computer-generated optimal design, as modified by additional requirements such as the total number of fuels and specific properties for subsets of fuels. In addition, to generate the design, it was necessary to specify the fuel effects to be estimated by the resulting model. The fuel set was designed to allow estimation of linear effects for the five properties shown in Table 6-2, plus two-way interactions of ethanol and the other five properties, as shown in Equation 6-1, in which β represents a linear coefficient for each effect.

$$\begin{aligned}
 Y = & \beta_0 + \beta_1\text{etOH} + \beta_2\text{Arom} + \beta_3\text{RVP} + \beta_4\text{T50} + \beta_5\text{T90} + \\
 & \beta_6\text{T50}^2 + \beta_{11}\text{etOH}^2 \\
 & \beta_7\text{etOH} \times \text{Arom} + \beta_8\text{etOH} \times \text{RVP} + \beta_9\text{etOH} \times \text{T50} + \beta_{10}\text{etOH} \times \text{T90} + \\
 & \varepsilon
 \end{aligned}
 \tag{Equation 6-1}$$

In the equation, the linear terms (e.g., $\beta_1\text{etOH}$, etc.) describe linear associations between emissions (Y) and the value of the fuel property. The quadratic terms are used to describe some degree of curvature in the relationship between emissions and the fuel property. Note that a minimum of 3 test levels for a property is needed to assess curvilinear relationships and that the design included such effects only for ethanol and T50. Two-way interaction terms indicate that the relationship between emissions and the first fuel property is dependent on the level of the second fuel property. For example, if an $\text{etOH} \times \text{Arom}$ interaction is included in a model, it implies that the effect of ethanol on the emission Y cannot be estimated without accounting for the aromatics level, and vice versa.

Using start NO_x as an example, we can use the relationship between emissions, ethanol and aromatics levels as an example. Figure 6-1(a) shows $\ln\text{NO}_x$, averaged by nominal ethanol levels. Different series are shown for means at the high and low aromatics levels and across both levels (“linear effect”). The linear effect would suggest a small but positive coefficient for ethanol. However, accounting for the ethanol level shows a more complex relation in which the trend at low aromatics is steeper than the linear effect, and that the effect at high aromatics inverts from a positive to negative slope. Similarly, in Figure 6-1(b), the complementary view is shown, with mean $\ln\text{NO}_x$ vs. aromatics levels, and with separate series for the three ethanol levels and across all levels. The trends are marked and positive in all cases, but with steepness decreasing with increasing ethanol level. The overall mean or “linear effect” is very close to the middle ethanol level (10 vol.%). Overall, this relationship can be characterized as an “interference interaction” in that increasing the level of aromatics reduces the steepness of the trend with ethanol, and vice versa. Note also that in (a), a slight curvature in the trends suggests that a quadratic term for ethanol could be appropriate. In fact, the quadratic term is not significant in fitting this model, whereas the interaction is found to be significant.

Figure 6-1. NO_x (Bag 1): Mean emissions levels, averaged by three ethanol and two Aromatics Levels, depicting an etOH×Arom interaction.



Note that inclusion of the 11 effects in the design does not imply that all effects will be retained in all models following the fitting process. Properties for each of the test fuels are shown in Table 6-3.

In conducting measurements, the LA92 “Unified” test cycle was used with emissions measured over three phases analogous to those in the Federal Test Procedure (FTP), at an ambient temperature of 75°F. The three phases (“bags”) of the cycle are characterized as “cold-start” (bag 1), “hot-running” (bag 2) and “hot-start” (bag 3). In the discussion that follows, the terms “cold-start,” “start” and “bag 1” will be treated as effectively synonymous. Similarly, the terms “hot-running,” “running” and “bag 2” will be treated as synonymous.

Note that in MOVES, the EPAAct results are applied at temperatures higher and lower than this level, under an assumption that effects for fuels and temperature are independent and multiplicative.

Emissions measured include carbon dioxide (CO₂), carbon monoxide (CO), total hydrocarbons (THC), methane (CH₄), oxides of nitrogen (NO_x), and particulate matter (PM_{2.5}). In addition, hydrocarbons were speciated for subsets of vehicles and fuels, allowing calculation of derived parameters such as non-methane organic gases (NMOG) and non-methane hydrocarbons (NMHC). Speciation also allowed independent analyses of selected toxics including acetaldehyde, formaldehyde, acrolein, benzene and 1,3-butadiene.

Phase 3 data collection was completed in June 2010. Dataset construction and analysis was conducted between January 2010 and November 2012. This process involved ongoing collaboration among EPA staff, DOE staff and contractors, and CRC representatives. Following the completion of data collection, construction of the dataset involved intensive evaluation and quality assurance. The analysis was iterative, with some steps triggering additional physical and chemical review of the data.

Successive rounds of statistical modeling were applied to the data, to achieve several goals, including identification of potential candidate models, identification and review of outlying observations, identification and review of subsets of data from influential vehicles, and identification of models including subsets of terms that best explain the results obtained. The process is briefly described in the following section.

The EPAAct exhaust research program and analysis are extensively documented in the “EPAAct Test Program Report”⁴¹ and “EPAAct Analysis Report.”⁴² This chapter describes how the

statistical models developed during the EAct study are applied in the MOVES model (MOVES2014).

Table 6-3. Measured Parameters for Fuels in the Phase-3 EAct Program.

Fuel ¹	etOH (vol.%)	Aromatics (vol.%)	RVP (psi) ²	T50 (°F)	T90 (°F)
1	10.03	15.4	10.07	148.9	300.2
2	0	14.1	10.2	236.7	340.1
3	10.36	15.0	6.93	217.5	295.9
4	9.94	15.5	10.01	221.9	337.5
5	0	34.7	6.95	237.0	300.0
6	10.56	15.0	7.24	188.5	340.4
7	0	17.0	7.15	193.1	298.4
8	0	15.7	10.2	221.1	303.1
9	0	35.8	10.30	192.8	341.8
10	9.82	34.0	7.11	217.1	340.2
11	10.30	35.0	9.93	189.3	298.6
12	9.83	34.8	10.13	152.2	339.8
13	0	34.1	6.92	222.5	337.9
14	0	16.9	7.14	192.8	338.5
15	0	35.3	10.23	189.7	299.4
16	10.76	35.6	7.12	218.8	300.6
20	20.31	15.2	6.70	162.7	298.7
21	21.14	35.5	7.06	167.6	305.0
22	20.51	15.0	10.21	163.2	297.3
23	20.32	15.9	6.84	162.5	338.2
24	20.51	15.3	10.12	165.1	338.1
25	20.03	35.2	10.16	166.9	337.9
26	15.24	35.6	10.21	160.3	338.7
27	14.91	14.9	6.97	221.5	340.3
28	14.98	34.5	6.87	216.6	298.8
30	9.81	35.5	10.23	152.9	323.8
31	20.11	35.5	6.98	167.3	325.2

¹ Note that numbering of fuels is not entirely sequential throughout.

² This parameter was measured as “DVPE,” but for simplicity, will be referred to as “RVP” in this document.

6.2 Analysis and Model Fitting

This chapter concerns the development and application of models for four pollutants (THC, CO, NO_x and PM) and two test phases, i.e., start (bag1) and running (bag 2). For all models, the response variable was the natural logarithm of cycle aggregate emissions on a single test phase of the LA92 cycle (g/mi for gaseous emissions, mg/mi for particulate). The predictor variables were the 11 fuel properties terms, “centered” and “scaled” as described in the next sub-section.

6.2.1 Standardizing Fuel Properties

In applying the EPAct models to estimate emissions effects for a given fuel, it is necessary to first “center” and “scale” the properties for the fuel, a process also known as “standardization.” This process simply involves first “centering” the measured fuel properties by subtracting the given value from the sample mean, and then “scaling” by then dividing the centered values by their respective standard deviations (with the means and standard deviations calculated from the fuel set used in the study), as shown in Equation 6-1. The result is a “Z score,” representing a “standard normal distribution” with a mean of 0.0 and a standard deviation of 1.0.⁴³

$$Z_i = \frac{x_i - \bar{x}}{s} \quad \text{Equation 6-2}$$

For the linear effects in the model, standardization is performed using the values of each fuel property, each in their respective scales (vol. %, psi, °F.). Using aromatics as an example, the standardization of the linear term is shown in Equation 6-3.

$$Z_{\text{arom}} = \frac{x_{\text{arom}} - \bar{x}_{\text{arom}}}{s_{\text{arom}}} \quad \text{Equation 6-3}$$

For second-order terms, however, the process is not performed on the values of the fuel properties themselves. Rather, quadratic and interaction terms are constructed from the Z scores for the linear terms, and the process is repeated. This step is taken to neutralize correlations between second-order terms and the linear terms from which they were constructed. Using the quadratic term for ethanol as an example (etOH×etOH), the standardized value, denoted by ZZ_{etOH×etOH}, is calculated as shown in Equation 6-4, where $m_{Z_{\text{etOH}}Z_{\text{etOH}}}$ and $s_{Z_{\text{etOH}}Z_{\text{etOH}}}$ are the mean and standard deviation of the quadratic term constructed from the Z score for the linear effect.

$$ZZ_{\text{etOH}\times\text{etOH}} = \frac{Z_{\text{etOH}}Z_{\text{etOH}} - m_{Z_{\text{etOH}}Z_{\text{etOH}}}}{s_{Z_{\text{etOH}}Z_{\text{etOH}}}} \quad \text{Equation 6-4}$$

Standardized terms for interaction effects are constructed similarly. For example, Equation 6-5 shows the standardization of an interaction term between ethanol and aromatics.

$$ZZ_{\text{etOH} \times \text{Arom}} = \frac{Z_{\text{etOH}} Z_{\text{Arom}} - m_{Z_{\text{etOH}} Z_{\text{Arom}}}}{s_{Z_{\text{etOH}} Z_{\text{Arom}}}} \quad \text{Equation 6-5}$$

Means and standard deviations for relevant model terms designs are shown in Table 6-4. Note that the means and standard deviations shown in the table are calculated from the fuel set itself as shown in Table 6-3; in this calculation the properties are not weighted for numbers of replicates on each fuel and emission combination. In this way, the process is simplified by using the same standardization in fitting all models, as well as in subsequent application of the models.

The process of standardization is illustrated for a fuel in Table 6-5, taking Tier-3 Certification fuel as an example. Overall, the process applied here is similar to the “correlation transformation” sometimes applied in multiple regression. One difference in this case is that the standardization is applied only to the predictor variables, whereas it is also possible to apply it to the response variable.⁴⁴

Table 6-4. Means and Standard deviations for Fuel Properties, based on Fuel Set for the EPA Act Phase-3 Project.¹

Model Term	Mean	Standard deviation
Ethanol (vol.%)	10.3137	7.87956
Aromatics (vol.%)	25.6296	10.0154
RVP (psi)	8.5178	1.61137
T50 (°F)	190.611	28.5791
T90 (°F)	320.533	19.4801
etOH × etOH	0.962963	0.802769
T50 × T50	0.962963	0.739766
etOH × Arom	-0.03674	0.978461
etOH × RVP	-0.0992352	0.999615
etOH × T50	-0.541342	0.769153
etOH × T90	0.0163277	0.972825
¹ Applies to models fit with data from 13-15 vehicles measured on 27 fuels.		

Table 6-5. Example of One-Stage and Two-Stage Standardization for Tier-3 Certification fuel.¹

Fuel	etOH (vol.%)	Arom (vol.%)	RVP (psi)	T50 (°F)	T90 (°F)	etOH × etOH	T50 × T50	etOH × Arom	etOH × RVP	etOH × T50	etOH × T90
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Fuel properties

T3	9.8	23	8.95	200	325
Mean ²	10.31	25.63	8.518	190.6	320.5
Std. Dev. ³	7.880	10.02	1.611	28.58	19.48

One-Stage standardized values (Z) (Equation 6-3)

	Z _e	Z _a	Z _r	Z ₅	Z ₉						
T3	-0.06519	-0.2626	0.2682	0.3285	0.2293						
Mean ²						0.9630	0.9630	-0.03674	-0.09924	-0.5413	0.01633
Std. Dev. ³						0.8028	0.7398	0.9785	0.9996	0.7692	0.9728

Two-stage standardized values (ZZ) (Equation 6-4, Equation 6-5)

	ZZ _{ee}	ZZ ₅₅	ZZ _{ea}	ZZ _{er}	ZZ _{e5}	ZZ _{e9}
T3	-1.281	-1.657	0.3117	0.427923	1.001927	-0.01678

¹ See 79 FR 23528. Values assigned as midpoints of ranges; with RVP values for "General Testing."

² Mean and standard deviations of fuel properties for the entire fuel set. See Table 6-4.

³ Means and standard deviations of 2nd-order terms for the entire fuel set.

6.2.2 Fitting Procedures

Throughout model fitting, the response variable was the natural logarithm transformation of the emissions results (lnY), and the predictor variables were the one- or two-stage standardized fuel properties, as shown in Table 6-5. Thus, the model to be fit includes some subset of the 11 candidate terms, as shown in Equation 6-6.

$$\begin{aligned}
 \ln Y = & \beta_0 + \\
 & \beta_1 Z_e + \beta_2 Z_a + \beta_3 Z_r + \beta_4 Z_5 + \beta_5 Z_9 + \\
 & \beta_6 ZZ_{55} + \beta_7 ZZ_{ee} + \\
 & \beta_8 ZZ_{ea} + \beta_9 ZZ_{er} + \beta_{10} ZZ_{e5} + \beta_{11} ZZ_{e9} + \\
 & \varepsilon
 \end{aligned}
 \tag{Equation 6-6}$$

A model containing all 11 candidate terms is referred to as a “full model,” whereas a model containing a subset of the 11 terms is referred to as a “reduced model.” The goal of model fitting is to identify a reduced model by removing terms from the full model that do not contribute to fit.

Models for gaseous emissions (HC/CO/NO_x) were fit as “mixed models,” in which the terms listed in Equation 6-6 were included as “fixed” terms. In addition, a “random intercept” was fit for each vehicle, which represents the high degree of variability contributed to the dataset by

variability among the vehicles measured. One way of understanding this distinction that the fuel properties are “fixed” because the goal of the analysis is to estimate the effect of these parameters on the mean levels of emissions for the entire fleet. On the other hand, “vehicle” is treated as a “random” factor because the sample of vehicles measured is but one of many samples that could have been measured. In the analysis, the emission levels of the specific vehicles are not of interest *per se*, but rather the degree of variability contributed to the analysis by the different vehicles. Analyses were performed using the MIXED procedure in the Statistical Analysis System (SAS®), version 9.2.⁴⁵

Models for particulate matter were fit by “Tobit regression.” This technique was used because the datasets for PM were affected by low-end “censoring.” For measurements with low masses on the filter, the mass ostensibly obtained from the vehicle exhaust was lower than that accumulated from levels of background PM. In these cases, we assumed that a small but detectable PM mass was not measured accurately due to limitations in the sampling technique. In the Tobit technique, the fitting method (maximum likelihood) is modified so as to compensate for the absence of the censored measurements. As with the mixed models, individual intercepts were fit for each vehicle, however, that Tobit procedure does not distinguish “fixed” and “random” factors, vehicles were entered into the model as fixed factors. The Tobit models were fit using the LIFEREG procedure in SAS 9.2.⁴⁶

The process of model fitting proceeded through several iterations. An initial round of fitting was performed to identify influential observations. For this purpose, full models were used, with no model fitting performed. Observations were identified as “influential” if their “externally-deleted” residual was greater than 3.5 or less than -3.5.⁴⁷ This analysis is described in Section 5.2 of the Project Report.

A second round was then performed to identify sets of preliminary “reduced” models, i.e., models containing subsets of the 11 terms included in the design, identified as contributing to the fit to the dataset for specific pollutant×bag combinations. This process is described in Section 5.3 of the Project Report.

The results of the second round were designated as “preliminary reduced models.” These models were then used to identify influential vehicles, as described in Section 5.5 of the Project Report. Subsequent review of data for vehicles found to be highly influential for specific models led to additional scrutiny of these subsets of data and eventual exclusion of data for selected vehicles for specific models. The criterion for exclusion was that most measurements for a given vehicle were below levels of background contamination for the pollutant under consideration. Models thus affected were Bag-1 NO_x, Bag-2 NO_x and Bag-2 THC. The additional data review following influence analysis is described in Chapter 6 of the Project Report.

In a third and final round of model-fitting, final reduced or “best-fit” models were obtained, incorporating the results of the previous rounds and following the procedures described below. The outcome of the process was a set of “best fit” models, summarized in Chapter 7 of the project report and applied in MOVES (as described in sub-section 9.2.2 and the Executive Summary).

Models for the gaseous emissions (THC, CO, NO_x) were fit by following the a series of steps: (1) all possible candidate models were fit, and ranked by a goodness-of-fit criterion known as the “Bayesian Information Criterion” (BIC). (2) From the top set of 5-9 leading candidate models,

all terms were pooled, to form a starting model for next step. (3) a final fitting process was conducted by backwards elimination, in which all terms in the pool were included at the outset. In fitting successive models, terms not contributing to fit were removed based on results of likelihood-ratio tests.⁴⁴ Note that the BIC and LRT were used for model ranking and selection because all models were fit using “maximum-likelihood” (rather than “least-squares”) methods. Results for full and reduced models are shown in Table 6-6 through Table 6-11 for HC, CO and NO_x, respectively. In the tables, p denotes the number of parameters in the model, including the intercept, and BIC denotes the Bayesian Information Criterion. The models are ranked by BIC, with smaller values indicating a better fit to the data.

Models for particulate matter were not fit by the process described in the previous paragraph but simply by backwards elimination starting with the 11 terms in the study design. Results for these models are shown in Table 6-12 and Table 6-13.

Table 6-6. THC (Bag 1): Coefficients and Tests of Effect for the Full and Reduced Models, with BIC = 263.09 and 260.63, respectively. Note that the 11 terms in the Full Model include those in the top five candidate models, as ranked by BIC.

Effect	<i>Full Model (superset)</i>					<i>Reduced Model (SM1)</i>				
	Estimate	Std. Err.	d.f.	t-value	Pr>t	Estimate	Std. Err.	d.f.	t-value	Pr>t
Intercept	-0.8663	0.0944	15	-9.18	0.00000	-0.8664	0.0944	15	-9.18	0.00000
Z _ε	0.0555	0.0127	941	4.36	0.00001	0.0548	0.0127	941	4.33	0.00002
Z _α	0.0678	0.0089	941	7.64	0.00000	0.0676	0.0089	941	7.62	0.00000
Z _γ	-0.0439	0.0101	941	-4.33	0.00002	-0.0445	0.0101	941	-4.43	0.00001
Z _δ	0.1296	0.0128	941	10.14	0.00000	0.1288	0.0127	941	10.15	0.00000
Z _ρ	0.0178	0.0089	941	2.01	0.04481	0.0183	0.0088	941	2.07	0.03898
ZZ _{εε}	0.0452	0.0171	941	2.64	0.00834	0.0436	0.0168	941	2.60	0.00959
ZZ _{δδ}	0.0742	0.0128	941	5.80	0.00000	0.0736	0.0128	941	5.77	0.00000
ZZ _{αα}	0.0183	0.0087	941	2.11	0.03542	0.0179	0.0087	941	2.07	0.03857
ZZ _{γγ}	0.0044	0.0089	941	0.50	0.61726					
ZZ _{εδ}	0.0460	0.0183	941	2.51	0.01227	0.0445	0.0181	941	2.46	0.01409
ZZ _{ερ}	0.0208	0.0087	941	2.38	0.01729	0.0214	0.0086	941	2.49	0.01294
σ_{veh}^2	0.1325					σ_{veh}^2	0.1325			
σ_{τ}^2	0.06870					σ_{τ}^2	0.06872			

Table 6-7. THC (Bag 2): Coefficients and Tests of Effect for the Full and Reduced Models, with BIC = 226.11 and 224.30, respectively. Note that the 10 terms in the Full Model include those in the top five candidate models, as ranked by BIC. These models were fit without the Siena and Odyssey.

Effect	<i>Full Model (superset)</i>					<i>Reduced Model (SM3)</i>				
	Estimate	Std. Err.	d.f.	t-value	Pr>t	Estimate	Std. Err.	d.f.	t-value	Pr>t
Intercept	-4.6543	0.2545	13	-18.29	0.0000	-4.6533	0.2541	13	-18.31	0.00000
Z _ε	0.0331	0.0120	819	2.77	0.0057	0.0327	0.0120	819	2.73	0.0066
Z _α	-0.0194	0.0093	819	-2.09	0.0370	-0.0195	0.0093	819	-2.10	0.0360
Z _γ	-0.0354	0.0106	819	-3.33	0.0009	-0.0355	0.0106	819	-3.36	0.00080
Z _δ	0.0476	0.0129	819	3.69	0.0002	0.0501	0.0129	819	3.89	0.0001
Z _ρ	0.0506	0.0094	819	5.39	0.0000	0.0514	0.0093	819	5.54	0.00000
ZZ _{εε}	-----					-----				
ZZ _{δδ}	0.0334	0.0094	819	3.55	0.0004	0.0337	0.0094	819	3.59	0.00036
ZZ _{αα}	0.0121	0.0091	819	1.33	0.1839					
ZZ _{γγ}	-0.0121	0.0092	819	-1.31	0.1914					
ZZ _{εδ}	-----					-----				
ZZ _{ερ}	-0.0116	0.0092	819	-1.2600	0.2080					
σ_{veh}^2	0.8406					σ_{veh}^2	0.8384			
σ_{τ}^2	0.06669					σ_{τ}^2	0.06717			

Table 6-8. CO (Bag 1): Coefficients and Tests of Effect for the Full and Reduced Models, with BIC = 324.99 and 322.48, respectively. Note that the 11 terms in the Full Model include those in the top six candidate models, as ranked by BIC.

Effect	<i>Full Model (Superset)</i>					<i>Reduced Model (SM1)</i>				
	Estimate	Std.Err.	d.f.	t-value	Pr> t	Estimate	Std.Err.	d.f.	t-value	Pr> t
Intercept	1.3467	0.1618	15	8.32	<0.0001	1.3466	0.1619	15	8.32	<0.0001
Z _e	-0.1051	0.01305	941	-8.06	<0.0001	-0.1049	0.01304	941	-8.05	<0.0001
Z _a	-0.01248	0.009092	941	-1.37	0.170	-0.01242	0.009092	941	-1.37	0.172
Z _r	-0.0081	0.01038	941	0.780	0.436	-0.00762	0.01033	941	-0.737	0.461
Z ₅	-0.03285	0.01310	941	-2.51	0.0123	-0.03273	0.01310	941	-2.50	0.0126
Z ₉	-0.1565	0.009095	941	17.20	<0.0001	-0.1571	0.008992	941	-17.47	<0.0001
ZZ _{ee}	0.07290	0.01751	941	4.16	<0.0001	0.07304	0.01750	941	4.17	<0.0001
ZZ ₅₅	0.05362	0.01311	941	4.09	<0.0001	0.05358	0.01311	941	4.09	<0.0001
ZZ _{ea}	0.02074	0.008894	941	2.33	0.0199	0.02086	0.008891	941	2.35	0.0192
ZZ _{er}	0.01535	0.009073	941	1.69	0.0911	0.01596	0.008967	941	1.78	0.0753
ZZ _{e5}	0.1062	0.01879	941	5.65	<0.0001	0.1064	0.01878	941	5.67	<0.0001
ZZ _{e9}	0.003963	0.008928	941	0.444	0.657			941		

σ_{veh}^2	0.3917	0.3920
σ_{ε}^2	0.07212	0.07214

Table 6-9. CO (Bag 2): Coefficients and Tests of Effect for the Full and Reduced Models, with BIC = 857.84 and 851.62, respectively. Note that the Eight terms in the Full Model include those in the top 8 candidate models, as ranked by BIC.

Effect	<i>Full Model (superset)</i>					<i>Reduced Model (SM4)</i>				
	Estimate	Std. Err.	d.f.	t-value	Pr>t	Estimate	Std. Err.	d.f.	t-value	Pr>t
Intercept	-1.3899	0.3578	15	-3.88	0.0015	-1.3893	0.3578	15	-3.88	0.0015
Z _e	0.01949	0.01567	941	1.24	0.21					
Z _a	0.09453	0.01195	941	7.91	0.00000	0.0913	0.0118	941	7.76	0.0000
Z _r	0.03769	0.01351	941	2.79	0.0054	0.0299	0.0122	941	2.45	0.0144
Z ₅	0.03936	0.01655	941	2.38	0.018	0.0261	0.0123	941	2.12	0.0342
Z ₉	0.04214	0.01190	941	3.54	0.00042	0.0440	0.0118	941	3.73	0.0002
ZZ _{ee}	0.01713	0.01220	941	1.40	0.16					
ZZ ₅₅	-0.003339	0.01205	941	-0.277	0.78					
ZZ _{ea}	---	---	---	---	---					
ZZ _{er}	---	---	---	---	---					
ZZ _{e5}	---	---	---	---	---					
ZZ _{e9}	-0.01487	0.01161	941	-1.28	0.20					

σ_{veh}^2	1.9182	σ_{veh}^2	1.9187
σ_r^2	0.1250	σ_r^2	0.1256

Table 6-10. NO_x (Bag 1): Coefficients and Tests of Effect for the Full and Reduced Models, with BIC = 914.04 and 911.00, respectively. Models were fit without the Ford Focus. Note that the six terms in the Full Model include those in the top six candidate models, as ranked by BIC.

Effect	<i>Full Model (Superset)</i>					<i>Reduced Model (SM2)</i>				
	Estimate	Std.Err.	d.f.	<i>t</i> -value	Pr> <i>t</i>	Estimate	Std.Err.	d.f.	<i>t</i> -value	Pr> <i>t</i>
Intercept	-2.8598	0.2061	14	-13.87	<0.0001	-2.8594	0.2061	14	-13.87	<0.0001
Z _e	0.06830	0.01688	879	4.05	<0.0001	0.06750	0.01568	879	4.30	<0.0001
Z _a	0.1368	0.01333	879	10.27	<0.0001	0.1339	0.01320	879	10.15	<0.0001
Z _r	---	---	---	---	---	---	---	---	---	---
Z ₅	0.04678	0.01688	879	2.77	0.0057	0.04783	0.01619	879	2.95	0.0032
Z ₉	---	---	---	---	---	---	---	---	---	---
ZZ _{ee}	0.00634	0.01899	879	0.334	0.74	---	---	---	---	---
ZZ ₅₅	---	---	---	---	---	---	---	---	---	---
ZZ _{ea}	-0.02343	0.01302	879	-1.80	0.072	-0.02369	0.01290	879	-1.84	0.067
ZZ _{er}	---	---	---	---	---	---	---	---	---	---
ZZ _{e5}	-0.01495	0.01857	879	-0.805	0.42	---	---	---	---	---
ZZ _{e9}	---	---	---	---	---	---	---	---	---	---

σ_{veh}^2	0.5926
σ_{ε}^2	0.1454

0.5925
0.1458

Table 6-12. PM (Bag 1): Coefficients and Tests of Effect for the Full and Reduced Models.

Effect	<i>Full Model</i>					<i>Reduced Model (FM6)</i>				
	Estimate	Std. Err.	d.f.	χ^2 - value	$Pr>\chi^2$	Estimate	Std. Err.	d.f.	χ^2 - value	$Pr>\chi^2$
Intercept ¹						0.6559				
Z_e	0.1365	0.05030	1	7.35	0.0067	0.1582	0.04130	1	14.7	0.00010
Z_a	0.3840	0.03510	1	119.96	<.0001	0.3833	0.03480	1	121	<.0001
Z_r	-0.0227	0.04000	1	0.32	0.57					
Z_5	0.0338	0.05050	1	0.45	0.50	0.0550	0.04310	1	1.63	0.20
Z_9	0.2965	0.03510	1	71.48	<.0001	0.2923	0.03440	1	72.2	<.0001
ZZ_{ee}	-0.0401	0.06750	1	0.35	0.55					
ZZ_{55}	0.0700	0.05050	1	1.92	0.166	0.0935	0.03420	1	7.46	0.0063
ZZ_{ea}	0.0508	0.03430	1	2.19	0.139					
ZZ_{er}	0.0295	0.03500	1	0.71	0.40					
ZZ_{e5}	-0.0482	0.07230	1	0.44	0.51					
ZZ_{e9}	0.0503	0.03440	1	2.14	0.14					
σ_{veh}^2 ¹						0.4251				
σ_ε^2	1.0321					1.0359				

¹ Not fit by Tobit model; calculated manually from individual vehicle intercepts.

Table 6-13. PM(Bag 2): Coefficients and Tests of Effect for the Full and Reduced Models.

Effect	<i>Full Model</i>					<i>Reduced Model (FM8)</i>				
	Estimate	Std. Err.	d.f.	χ^2 - value	$Pr>\chi^2$	Estimate	Std. Err.	d.f.	χ^2 - value	$Pr>\chi^2$
Intercept ¹						-1.3107				
Z_e	0.0390	0.0552	1	0.500	0.48	0.1126	0.0370	1	9.27	0.0023
Z_a	0.1619	0.0384	1	17.8	<.0001	0.1662	0.0376	1	19.6	<.0001
Z_r	-0.0615	0.0438	1	1.97	0.16					
Z_5	-0.0725	0.0553	1	1.72	0.19					
Z_9	0.1064	0.0384	1	7.69	0.0055	0.1072	0.0376	1	8.14	0.0043
ZZ_{ee}	-0.1380	0.0739	1	3.48	0.062					
ZZ_{55}	-0.0143	0.0553	1	0.0700	0.80					
ZZ_{ea}	0.0210	0.0375	1	0.31	0.58					
ZZ_{er}	-0.0272	0.0383	1	0.50	0.48					
ZZ_{e5}	-0.1109	0.0795	1	1.95	0.16					
ZZ_{e9}	-0.0135	0.0377	1	0.13	0.72					
σ_{veh}^2 ¹						0.7827				
σ_ε^2	1.1294					1.1337				

¹ Not fit by Tobit model; calculated manually from individual vehicle intercepts.

6.3 Scope and Implementation

Within MOVES, the steps described in this document are applied within the scope listed below.

Fuels: The adjustments apply to gasoline (fuelTypeID = 1) . The adjustments described in this document are applied to gasoline blends containing 0-15 vol.% ethanol.

Engine technology: For MOVES2014, these adjustments will apply to all engine technologies other than purely electric vehicles.

Model Years: Adjustments apply to model year 2001 and later.

SourceType: The adjustments apply to all sourceTypes.

Emission Processes: Adjustments are developed and applied separately to running exhaust (processID = 1) and start exhaust emissions (processID = 2).

Pollutants: The pollutants covered include those listed in Table 6-14.

Table 6-14. Pollutants Modified by Fuel Adjustments

pollutantID	pollutantName	Acronym
1	Total Gaseous Hydrocarbons	THC
2	Carbon Monoxide	CO
3	Oxides of Nitrogen (NO _x)	NO _x
112	Primary PM _{2.5} – Elemental Carbon	PM(EC) ²
118	Primary PM _{2.5} – non-Elemental Carbon	PM(nonEC) ²
20	Benzene	
21	Ethanol	
24	1,3-Butadiene	
25	Formaldehyde	
26	Acetaldehyde	
27	Acrolein	
² As the same adjustments are applied to OC and EC, they will be referred to more generically as “PM” in this document.		

Database Table: MOVES2014 allows a very flexible input data format for incorporating and applying coefficients within a wide variety of mathematical forms. These “fuel-effect ratio expressions” can include up to 32,000 characters and are stored in a database table dedicated to this purpose (*GeneralFuelRatioExpression*).

6.4 Fuel Effect Adjustments

In MOVES, emissions of the pollutants THC, CO, NO_x and PM are calculated starting with “base emission rates” (meanBaseRate, meanBaseRateIM) stored in the database table, emissionRateByAge.⁴⁸ The base rates are assumed to represent emissions on a “base fuel” which are multiplied by a ratio adjustment to represent emissions on a selected in-use fuel. Different fuel adjustments have been developed to represent selected pollutants and emission processes. Adjustments also vary depending on vehicle type and model year. This chapter describes the application of the EPAAct study results to derive fuel adjustments for the subsets of vehicles and model years described above.

The models generated using EPAAct results allow estimation of emissions effects related to five fuel properties: ethanol content (vol.%), aromatics content (vol.%), RVP (psi), T50 (°F) and T90 (°F), as well as selected interaction terms among these five parameters. The statistical models generated from the EPAAct exhaust data follow the general structure shown in Equation 6-7 below. Using the reduced model for cold-start NO_x as an example (see Table 6-10), β denotes a model coefficient, Z_{etOH} denotes a “standardized” fuel term for this property, and $Z_{\text{etOH}\times\text{Arom}}$ denotes a “standardized” etOH×Arom interaction term. Finally, the term s_e^2 represents the total error or “mean square error” for the model. Note that the model expression can be represented conveniently using the matrix notation “ $\mathbf{X}\beta$.”

$$\begin{aligned} \text{Emissions (g/mi)} &= \\ \exp\left(\beta_0 + \beta_{\text{etOH}}Z_{\text{etOH}} + \beta_{\text{Arom}}Z_{\text{Arom}} + \beta_{\text{T50}}Z_{\text{T50}} + \beta_{\text{etOH}\times\text{Arom}}Z_{\text{etOH}\times\text{Arom}} + 0.5s_e^2\right) & \text{Equation 6-7} \\ &= \exp(\mathbf{X}\beta) \end{aligned}$$

Relative fuel effects are calculated by applying the models to specific “in-use” fuels and pre-defined “base fuels” and by calculating the ratio of the emissions on the in-use fuel to those on the base fuel, as shown in Equation 6-8.

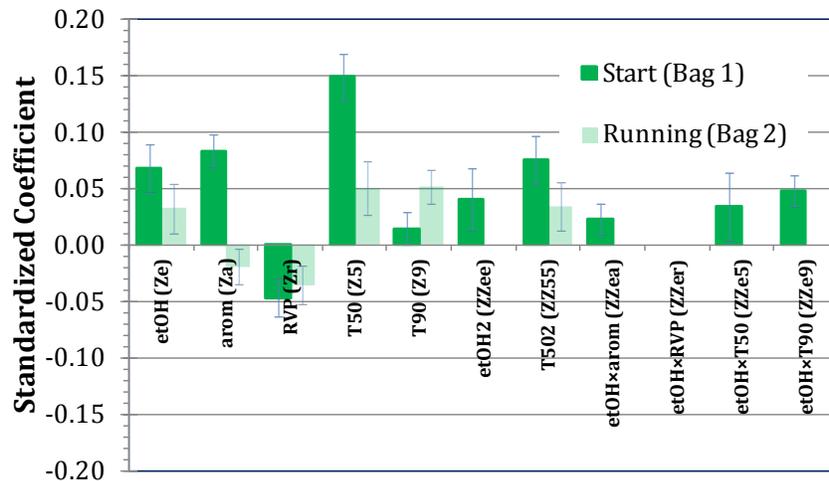
$$\text{Fuel Effect} = \frac{\exp(\mathbf{X}\beta_{\text{in-use}})}{\exp(\mathbf{X}\beta_{\text{base}})} = \exp(\mathbf{X}\beta_{\text{in-use}} - \mathbf{X}\beta_{\text{base}}) \quad \text{Equation 6-8}$$

The sets of coefficients for four individual pollutants, including total hydrocarbons (THC) and the criteria pollutants CO, NO_x, and PM have been presented in Table 6-6 through Table 6-13. The application of these models has been integrated into MOVES2014. For implementation in MOVES, this calculation is input directly into the *GeneralFuelRatioExpression* table.

The table presents two sets of coefficients for each pollutant, representing the effects of the fuel properties on start and running exhaust emissions, respectively.^b In some cases fuel effects estimated for these two processes differed substantially, as the effects of fuel properties on start emissions are dominated by changes in combustion and catalyst warm-up, while the effects on running emissions are dictated by catalyst efficiency when fully operational. These results are depicted graphically in Figure 6-2 through Figure 6-5, with the lengths and directions of the bars representing the magnitude and sign of coefficients, respectively.

The coefficients can be understood as the change in the natural logarithm of emissions (e.g., $\Delta \ln(\text{CO})$) associated with a change in the fuel property of 1.0 standard deviation, and assuming that *the other fuel properties remain constant*. Note that “standard deviation” refers to values defined for the fuel matrix used in the study (see Table 6-4). Because these coefficients apply to “standardized” fuel properties, as mentioned above, the magnitude and signs of the terms are comparable, giving a sense of the influence of each term in the estimation of that pollutant relative to the others. For example, for PM start emissions, changes in aromatics and T90 are very influential, and are positively related with PM emissions (e.g., when aromatics increase, PM increases). For THC start emissions, on the other hand, the negative sign of the RVP coefficient indicates that the relationship is inverse, i.e., increases in RVP are associated with decreases in THC.

Figure 6-2. THC: Standardized coefficients for models representing start and running emissions. (Error bars represent 90% confidence intervals for the coefficients).



^b For all models, “start” and “running” emissions are represented by results measured on Bags 1 and 2 of the LA92 cycle, respectively.

Figure 6-3. CO: Standardized coefficients for models representing start and running Emissions. (Error bars represent 90% confidence intervals for the coefficients).

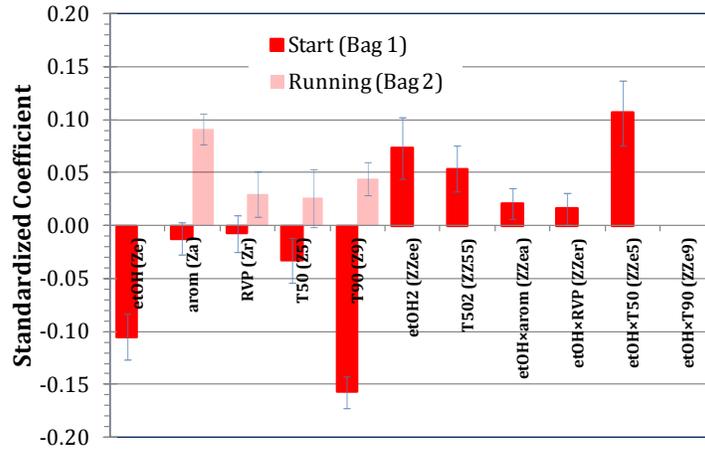


Figure 6-4. NOx: Standardized Coefficients for Models representing Start and Running Emissions. (Error bars represent 90% confidence intervals for the coefficients).

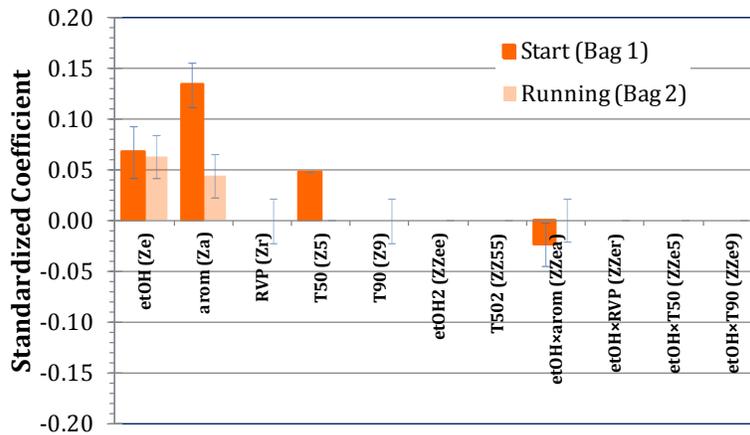
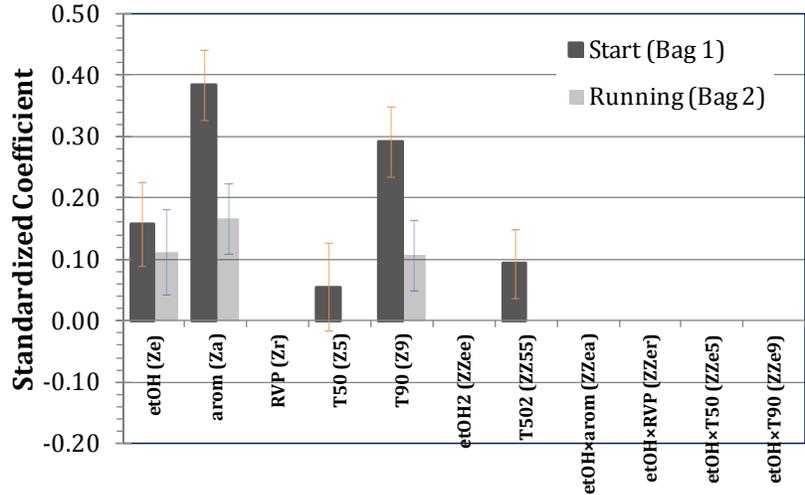


Figure 6-5. PM: Standardized Coefficients for Models representing Start and Running Emissions. (Error bars represent 90% confidence intervals for the coefficients).



6.5 The Database Table “GeneralFuelRatioExpression”

As mentioned, the models shown in Equations Equation 6-7 and Equation 6-8, applying coefficients as shown in Table 6-6 to Table 6-13, and in Figure 6-2 to Figure 6-5, are stored in the database table “GeneralFuelRatioExpression.” A description of this table is shown in Table 6-15.

Table 6-15. Description of the Database Table “GeneralFuelRatioExpression.”

Field	Description	Values
fuelTypeID	Identifies fuel types as broad classes, i.e., “gasoline,” “diesel,” etc.	1 = gasoline 2 = diesel, etc.
polProcessID	Identifies combinations of pollutant and process.	e.g., 301 = hot-running NO _x , etc.
minModelYearID	The earliest model year to which a specific value of fuelEffectRatioExpression is applied.	e.g., 2001
maxModelYearID	The latest model year to which a specific value of fuelEffectRatioExpression is applied.	e.g., 2050
minAgeID	The minimum vehicle age at which the value of fuelEffectRatioExpression is applied.	e.g., 0 years
maxAgeID	The maximum vehicle age at which the value of fuelEffectRatioExpression is applied.	e.g., 30 years
sourceTypeID	Identifies vehicles by functional type. See table “sourceUseType.”	11= motorcycle 21= passenger car 31=passenger truck 32=light commercial truck, etc.
fuelEffectRatioExpression	A mathematical expression containing up to 32,000 characters.	

6.5.1 Examples

We show an examples of the calculation of fuel adjustment for start NO_x applied in conjunction with the adjustment for fuel sulfur. Note that the adjustment for sulfur is calculated independently of that for the other properties: ethanol, aromatics, vapor pressure, T50 and T90. The calculation of adjustments for sulfur content is described in Chapter 3 in this document. The entire expression is shown below in Table 6-16. Due to its length, the whole is divided into terms and segments, which, along with descriptions, are presented in Table 6-17.

The calculations in the expression shown in Table 6-16 and Table 6-17 are shown in Table 6-18, which illustrates calculation of NO_x fuel adjustments for Tier-3 certification fuel, relative to a MOVES base fuel, although without the inclusion of the sulfur adjustment. Results are presented for both start and running models. Calculation of standardized fuel properties for the test fuels is illustrated in Table 6-5. The lower segments of the table present the model predictions, as ln(NO_x), NO_x rates as g/mi, obtained by exponentiating the logarithmic results, and the fuel adjustments, calculated as ratios of the rates for the test fuels to those for the base

fuel. As mentioned, note that the rates represent aggregate results on Bags 1 and 2 of the LA92 cycle, respectively.

For NO_x , the calculations predict increases of approximately 1.0% and 6.6% for start and running emissions, respectively. For THC, corresponding reductions for start and running emissions are 16.7% and 7.5%, respectively, as shown in Table 6-19 and Figure 6-7.

To understand how positive or negative changes in all five fuel properties affect the adjustment, it is useful to view the contributions of each model term. This step can be achieved by rearranging the calculation (for start NO_x) as shown in Equation 6-9 below. The rearrangement of terms shows that the adjustment can be calculated by applying the coefficients to the differences in standardized properties for the fuels to be compared. Note that the intercepts and variances drop out of the calculation.

$$\begin{aligned} \text{Fuel Adjustment} &= \exp(\mathbf{X}\boldsymbol{\beta}_{\text{in-use}} - \mathbf{X}\boldsymbol{\beta}_{\text{base}}) \\ &= \exp\left(\begin{array}{l} (\beta_0 + \beta_{\text{etOH}}Z_{\text{etOH,in-use}} + \beta_{\text{arom}}Z_{\text{arom,in-use}} + \beta_{\text{T50}}Z_{\text{T50,in-use}} + \beta_{\text{etOH}\times\text{Arom}}ZZ_{\text{etOH}\times\text{Arom,in-use}} + 0.5\sigma^2) - \\ (\beta_0 + \beta_{\text{etOH}}Z_{\text{etOH,base}} + \beta_{\text{arom}}Z_{\text{arom,base}} + \beta_{\text{T50}}Z_{\text{T50,base}} + \beta_{\text{etOH}\times\text{Arom}}ZZ_{\text{etOH}\times\text{Arom,base}} + 0.5\sigma^2) \end{array} \right) \\ &= \exp\left(\begin{array}{l} \beta_{\text{etOH}}(Z_{\text{etOH,in-use}} - Z_{\text{etOH,base}}) + \beta_{\text{arom}}(Z_{\text{arom,in-use}} - Z_{\text{arom,base}}) + \beta_{\text{T50}}(Z_{\text{T50,in-use}} - Z_{\text{T50,base}}) + \\ \beta_{\text{etOH}\times\text{Arom}}(ZZ_{\text{etOH}\times\text{Arom,in-use}} - ZZ_{\text{etOH}\times\text{Arom,base}}) \end{array} \right) \end{aligned}$$

Equation 6-9

Term-by-term results for the NO_x adjustments shown in Table 6-18 are presented graphically in Figure 6-6. Not surprisingly, these examples display the importance of the aromatics linear term. For the Tier-3 fuel, the ethanol term is positive, showing the effect of the increase in ethanol to 10 vol.% for the test fuel, relative to the base fuel. However, the positive ethanol term is almost entirely offset by the reductions in aromatics and T50.

Table 6-19 and Figure 6-7 show adjustments for start THC. The linear terms for ethanol, aromatics and T50 are directionally similar to those for NO_x in the previous example, but with the terms taking different sizes. In contrast to the picture for NO_x , the T50 linear term in combination with the two quadratic terms and the etOH×T50 interaction play important roles in the overall adjustment. Additionally, RVP plays a role in the THC adjustment, although relatively minor. Overall, the results give a negative adjustment for the certification fuel.

These examples make it clear that the net effect in emissions for one fuel relative to the base depends in changes in all properties in relation to each other. **Similarly, we must stress that the overall “effect” of any particular property, e.g., “the effect of aromatics on emissions,” cannot be simply inferred from the direction and size of its coefficient, taken in isolation. This point cannot be overemphasized in applying and interpreting the models.**

Table 6-16. Example Value for Field “fuelEffectRatioExpression” in Database Table “GeneralFuelRatioExpression” (NOTE: this example calculates an adjustment for cold-start NO_x, accounting for the fuel properties: ethanol, aromatics, vapor pressure, T50, T90 and sulfur).

```

if(sulfurLevel > 30,(exp(-2.8593506+(0.0675016*((ETOHVOLUME-
10.313704)/(7.879557)))+(0.1339309*((aromaticContent-
25.629630)/(10.015366)))+(0.0478207*((T50-190.611111)/(28.579112)))+(-
0.0236855*(((ETOHVOLUME-10.313704)/(7.879557))*((aromaticContent-25.629630)/(10.015366)))-
(-0.036738)/(0.978461))))*(1+((0.425*(exp(0.351*ln(303))-
exp(0.351*ln(30)))/exp(0.351*ln(30)))+0.575*(1.47*(exp(0.351*ln(sulfurLevel))-
exp(0.351*ln(30)))/exp(0.351*ln(30)))))/1.53198632576)/0.0552997544579),((exp(-
2.8593506+(0.0675016*((ETOHVOLUME-10.313704)/(7.879557)))+(0.1339309*((aromaticContent-
25.629630)/(10.015366)))+(0.0478207*((T50-190.611111)/(28.579112)))+(-
0.0236855*(((ETOHVOLUME-10.313704)/(7.879557))*((aromaticContent-25.629630)/(10.015366)))-
(-0.036738)/(0.978461))))/0.055299754458)*(1-0.0*(30-sulfurLevel))))

```

Table 6-17. Expression stored in the Field “fuelEffectRatioExpression” in the Table “GeneralFuelRatioExpression.”

Segment of Expression	Comments
if(sulfurLevel > 30 ,	Initiate condition to be applied for sulfur level > 30 ppm
(exp(-2.8593506 +	Initiate exponential expression, enter intercept for EPAct model.
(0.0675016*((ETOHVolume-10.313704)/(7.879557))) +	Enter standardized linear term for ethanol
(0.1339309*((aromaticContent-25.629630)/(10.015366))) +	Enter standardized linear term for aromatics
(0.0478207*((T50-190.611111)/(28.579112))) +	Enter standardized linear term for T50
(-0.0236855*(((ETOHVolume-10.313704)/(7.879557))*((aromaticContent-25.629630)/(10.015366)))-(-0.036738)/(0.978461)))) *	Enter standardized interaction term for ethanol×aromatics
((1+((0.425*(exp(0.351*ln(303))-exp(0.351*ln(30)))/exp(0.351*ln(30)))+0.575*(1.47*(exp(0.351*ln(sulfurLevel))-exp(0.351*ln(30)))/exp(0.351*ln(30)))))/1.53198632576)/0.0552997544579)	Apply expression to calculate sulfur effect (application of M6Sulf model).
,	Initiate else condition for sulfur Level <= 30 ppm. (NOTE: following comma, condition is implicit).
(exp(-2.8593506 +	Initiate exponential expression, enter intercept for EPAct model.
(0.0675016*((ETOHVolume-10.313704)/(7.879557))) +	Enter standardized linear term for ethanol
(0.1339309*((aromaticContent-25.629630)/(10.015366))) +	Enter standardized linear term for aromatics
(0.0478207*((T50-190.611111)/(28.579112))) +	Enter standardized linear term for T50
(-0.0236855*(((ETOHVolume-10.313704)/(7.879557))*((aromaticContent-25.629630)/(10.015366)))-(-0.036738)/(0.978461)))) *	Enter standardized interaction term for ethanol×aromatics
/0.055299754458)*(1-0.0*(30-sulfurLevel)))	Apply expression to estimate sulfur effect (T2 sulfur model).

Table 6-18. NO_x: Application of Models for Tier-3 Certification Fuel and a MOVES Base Fuel, with Calculation of Fuel Adjustments.

Fuel properties			Standardized properties			Models	
Property	Fuel		Model Term	Fuel		Coefficients	
	base	T3		base	T3	Start	Running
etOH (vol.%)	0	9.8	Z _e	-1.309	-0.06519	0.067502	0.062989
Arom (vol.%)	26.1	23	Z _a	0.04696	-0.2626	0.133931	0.044062
RVP (psi)	6.9	8.95	Z _r	-1.004	0.2682	0	0
T50 (°F)	218	200	Z ₅	0.9584	0.3285	0.047821	0
T90 (°F)	329	325	Z ₉	0.4346	0.2293	0	0
			ZZ _{ee}	0.9346	-1.194	0	0
			ZZ ₅₅	-0.0602	-1.156	0	0
			ZZ _{ea}	-0.02528	0.0550	-0.02369	0
			ZZ _{er}	1.414	0.08178	0	0
			ZZ _{e5}	-0.9271	0.6760	0	0
			ZZ _{e9}	-0.6016	-0.03215	0	0
			Intercept	1	1	-2.859	-4.569
			Variance			0.7383	0.6556
Results: start model							
			ln(NO _x)	-2.895	-2.884		
			NO _x (g/mi)	0.08002	0.08086		
			Adjustment	1.000	1.011		
Results: running model							
			ln(NO _x)	-4.649	-4.585		
			NO _x (g/mi)	0.01328	0.01417		
			Adjustment	1.000	1.067		

Figure 6-6. NO_x (Bag 1): Fuel Adjustment for Tier-3 Certification Fuel, Displayed by Individual Logarithmic Model Terms.

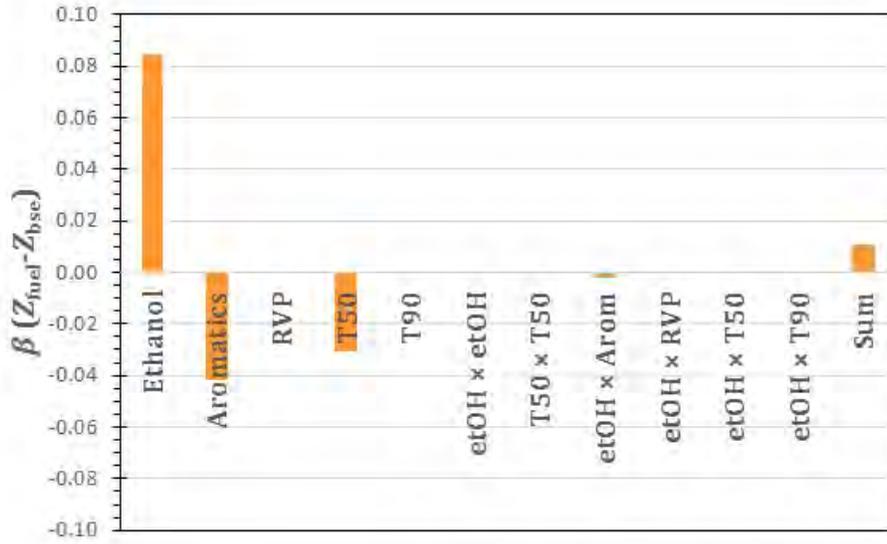
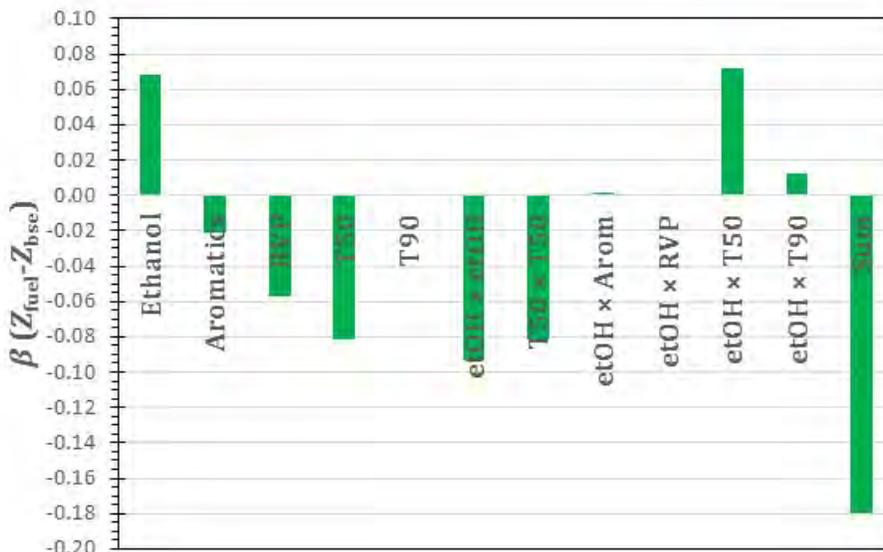


Table 6-19. THC: Application of Models for Tier-3 Certification Fuel and a MOVES Base Fuel, with Calculation of Fuel Adjustments.

Fuel properties			Standardized properties			Models	
Property	Fuel		Model Term	Fuel		Coefficients	
	base	T3		base	T3	Start	Running
etOH (vol.%)	0	9.8	Z_e	-1.309	-0.06519	0.05482	0.03268
Arom (vol.%)	26.1	23	Z_a	0.04696	-0.2626	0.06758	-0.01953
RVP (psi)	6.9	8.95	Z_r	-1.004	0.2682	-0.04453	-0.03553
T50 (°F)	218	200	Z_5	0.9584	0.3285	0.1288	0.05008
T90 (°F)	329	325	Z_9	0.4346	0.2293	0.01827	0.05136
			ZZ_{ee}	0.9346	-1.194	0.04361	0
			ZZ_{55}	-0.0602	-1.156	0.07364	0.03373
			ZZ_{ea}	-0.02528	0.0550	0.01792	0
			ZZ_{er}	1.414	0.08178	0	0
			ZZ_{e5}	-0.9271	0.6760	0.04446	0
			ZZ_{e9}	-0.6016	-0.03215	0.02145	0
			Intercept	1	1	-0.8664	-4.653
			Variance			0.2012	0.9056
Results: start model							
ln(THC)				-0.7771	-0.9600		
THC (g/mi)				0.5084	0.4234		
Adjustment				1.000	0.833		
Results: running model							
ln(THC)				-4.593	-4.670		
THC (g/mi)				0.01592	0.01474		
Adjustment				1.000	0.925		

Figure 6-7. THC (Bag 1): Fuel Adjustment for Tier-3 Certification Fuel, Displayed by Individual Logarithmic Model Terms.



7 High-Level Ethanol Blends (E85)

7.1 Introduction

Fuels containing 70 to 85 vol.% ethanol combined with hydrocarbon blendstocks (“E85”) have been available for many years and their use as transportation fuels has grown since passage of the Energy Policy Act of 2005 (EPAAct),⁴⁹ its implementation in the Renewable Fuel Standard (RFS)⁵⁰ and passage of the Energy Independence and Security Act of 2007 (EISA).⁵¹ Vehicles designed to run on gasoline or such “high-level” ethanol blends are designated as flexible-fuel or “flex-fuel” vehicles (FFVs). In the U.S., the highest ethanol blend that existing flex-fuel vehicles can use is E85.

With the increased use of E85 in the fleet, numerous studies have examined the differences in emissions of FFVs operated on E85 versus gasoline, typically E10. However, the numbers of vehicles included in these studies typically have been small and the results have been mixed in terms of the effects of E85 on emissions of gaseous or criteria-pollutant emissions from FFVs.^{52,53,54}

In MOVES2014, we have incorporated the capability of modeling emissions from vehicles running on E85. In MOVES2014, users can model E85 by selecting the “ethanol (E-85)” category⁵⁵ which includes fuels containing 70% or more ethanol by volume. MOVES2014 allows E85 use for the following sourceTypes only: passenger cars, passenger trucks, and light commercial trucks.⁵⁶

This chapter describes the analysis conducted to estimate the effects of E85 use on exhaust emissions of total hydrocarbons (THC), non-methane hydrocarbons (NMHC), non-methane organic gases (NMOG), carbon monoxide (CO), nitrogen oxides (NO_x), and particulate matter

(PM_{2.5}) from flex-fuel vehicles. The chapter also describes the underlying data used in the analysis, and the algorithms used to model the emissions from FFVs using E85 in MOVES2014. The MOVES2014 algorithms for estimating the effects of E85 on air toxics or evaporative hydrocarbons are discussed in separate reports.^{1,3}

7.2 Data Analysis and Results

The impacts of E85 on emissions on THC, NMHC, NMOG, CO, NO_x, and PM_{2.5} were examined using the results from four test programs, namely, the EPA Act Phase 3 program,⁵⁷ National Renewable Energy Laboratory (NREL) E40,⁵⁸ Coordinating Research Council (CRC) E-80,⁵⁹ and the EPA NRMRL Test Program.⁶⁰ The details of each program are described below.

Energy Policy Act (EPA Act) Program – Phase 3 of the EPA Act program included testing of four flexible-fuel vehicles on both E10 and E85 fuels. Table 7-1 shows the description of the tested vehicles. The vehicles were tested using the California Unified Cycle, also known as the LA92. The LA92 was conducted as a three-phase, cold start test similar to the FTP.

Table 7-1. Description of the Vehicles Tested in EPA Act Program.

Model Year	Make	Model	Odometer
2008	Chevrolet	Impala	5,048
2008	Chevrolet	Silverado	5,347
2008	Ford	F150	5,523
2008	Dodge	Caravan ¹	5,282

¹ Dodge Caravan was tested only on E85 fuel, and thus, was excluded from the analysis.

National Renewable Energy Laboratory (NREL) E40 – Nine flex-fuel vehicles aged between one and ten years were tested on three-phase LA92 cycles with a minimum of two replicates. Table 7-2 shows the description of the tested vehicles. The fuels examined in the study were a retail E10 meeting ASTM D4814 Class A-2 standards, a flex fuel containing 76 percent ethanol by volume, and a mid-level ethanol blend, E40. For the current analysis, only the data from vehicles running on E10 and E85 was included.

Table 7-2. Description of the Vehicles Tested in NREL E40 Program.

Model Year	Make	Model	Odometer
2011	GMC	Terrain	10,000
2010	Chrysler	Town & Country	28,000
2010	Toyota	Tundra	17,000
2009	Nissan	Titan	21,000
2011	Ford	Fusion	11,000
2007	Chevrolet	Silverado	10,000
2002	Ford	Taurus	115,000
2002	Dodge	Caravan	110,000
2002	Chevrolet	Tahoe	118,000

Coordinating Research Council (CRC) E-80 Project – This study conducted by the Coordinating Research Council tested seven flex-fuel vehicles running on four different ethanol blends (E6, E32, E59, and E85). The test vehicles (see Table 7-3) were driven under various test cycles – Cold Start Federal Test Procedure (FTP), Hot Start High Speed/Load Driving Cycle (US06), and Cold Start Unified Driving Cycle (LA92). Each vehicle, fuel, and test condition was measured only once. For the current analysis, only the data from vehicles running on E6 and E85 under LA92 cycle was included.

Table 7-3. Description of the Vehicles Tested in CRC E-80 Project.

Model Year	Make	Model	Odometer
2007	Dodge	Grand Caravan	30,514
2007	Ford	F-150 XLT	12,646
2007	Ford	Crown Victoria	16,345
2007	Chevrolet	Tahoe LS	18,555
2007	Chevrolet	Silverado LT	22,008
2007	Chevrolet	Uplander LS	17,898
2006	Chevrolet	Monte Carlo	48,761

EPA NRMRL Test Program (“PM Speciation Program”) – As part of a coordinated program between EPA/ORD/NRMRL (Research Triangle Park, NC) and EPA/OAR/OTAQ (Ann Arbor, MI), the study tested Tier 2 flex-fuel vehicles (see Table 7-4) running on E0, E10, and E85 driven under LA92 cycle run as a 4-phase test. The test cycle was repeated for each ethanol blend and vehicle. For the current analysis, only the data from vehicles running on E10 and E85 were included.

Table 7-4. Description of the Vehicles Tested in EPA NRMRL Test Program.

Model Year	Make	Model	Odometer
2008	Chevrolet	Impala	50,000
2008	Chrysler	Town & Country	50,000

All programs measured emissions on the LA92 cycle running on both E10 and E85 blends, except CRC E-80, which measured E6 and E85 blends. Table 7-5 describes the properties of the fuels used in each of the programs included in the current analysis. Only the vehicles tested on both E10 (E6) and E85 were included in the analysis. The composite emissions were calculated using the same weighting factors as specified for the FTP.

Table 7-5. Fuel Properties of the Fuels Used in Each Program.

Property	EPAAct		NREL E40		CRC E-80		EPA NRMRL	
	E10	E85	E10	E85	E6	E85	E10	E85
EtOH (vol.%)	10	77	10.6	75.5	6	82.9	9.3	80.5
Aromatics (vol.%)	26.2	5.9	20.8	7.1	11.9	2.0	21.8	5.7
RVP (psi)	8.8	8.9	8.4	5.8	7.3	7.3	9.2	8.9
T50 (°F)	189.7	171.8	160.0	172.2	204.2	171.3	221.0	171.5
T90 (°F)	319.7	173.9	307.8	174.2	307.8	172.5	325.2	173.5

Initially, each dataset was analyzed separately to examine the differences in emissions between E10 and E85. However, because the preliminary results showed directionally consistent emission trends across datasets and similar percent changes in emission between E10 and E85, all available datasets were pooled to examine the effect of E85 on emissions, relative to E10. We acknowledge that fuel properties other than ethanol are confounders and therefore, they may introduce bias to the extent that fuel properties of E10 and E85 vary between programs. However, considering the small sample size in each dataset, we believe performing Student's paired *t*-test on a pooled dataset increases the statistical power and reduces the effects of confounders, compared to an analysis that examines the effect of E85 on emissions compared to E10 for each test program. Because not all programs measured the same set of pollutants, the numbers of test vehicles included in the analysis are different for each pollutant (Table 7-6).

Table 7-6. Number of Vehicles for Analysis of Each Pollutant.

Pollutant	Number of Vehicles
THC	12
NMOG	19
NMHC	7
CH ₄	5
NO _x	21
PM _{2.5}	5
CO	21

Figure 7-1 through Figure 7-7 show the mean measured emissions for E10 and E85. The error bars represent the 95% confidence intervals.

Figure 7-1. Mean THC Emissions from Vehicles Running on E10 and E85.

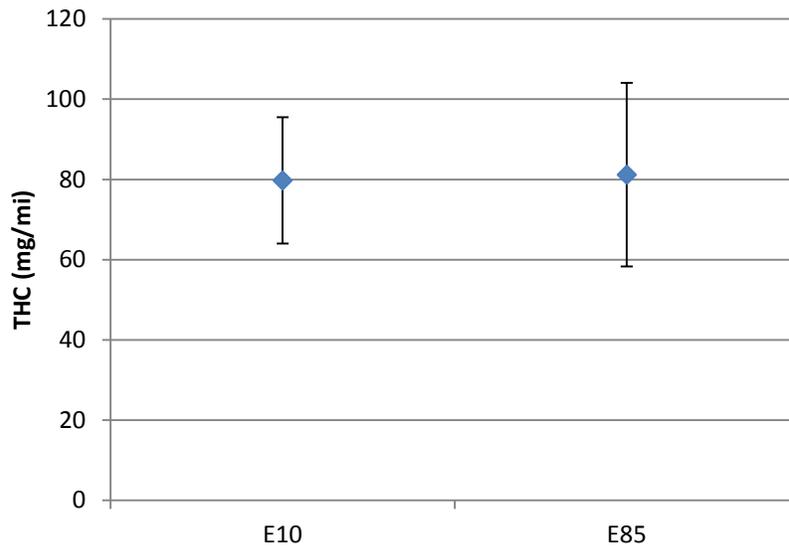


Figure 7-2. Mean NMOG Emissions from Vehicles Running on E10 and E85.

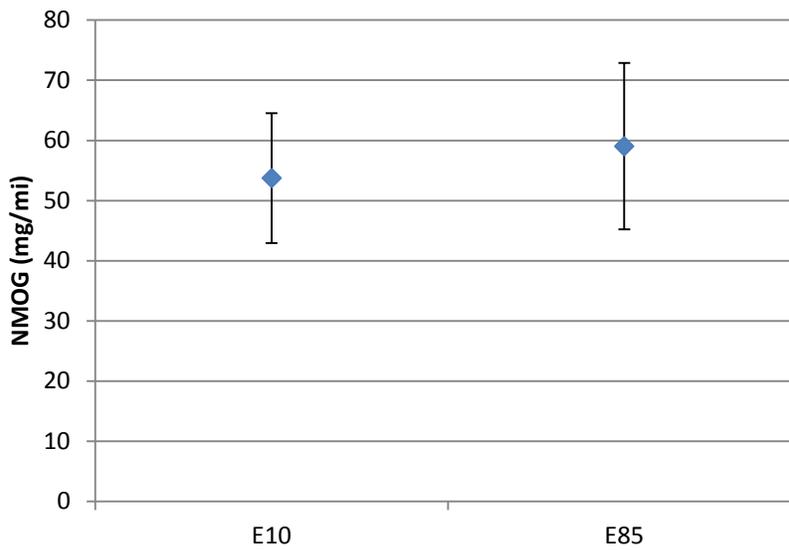


Figure 7-3. Mean NMHC Emissions from Vehicles Running on E10 and E85.

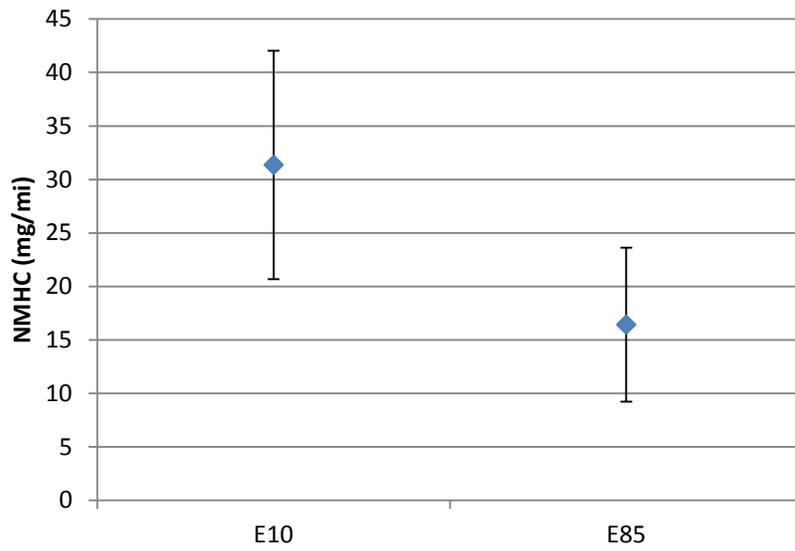


Figure 7-4. Mean CH₄ Emissions from Vehicles Running on E10 and E85.

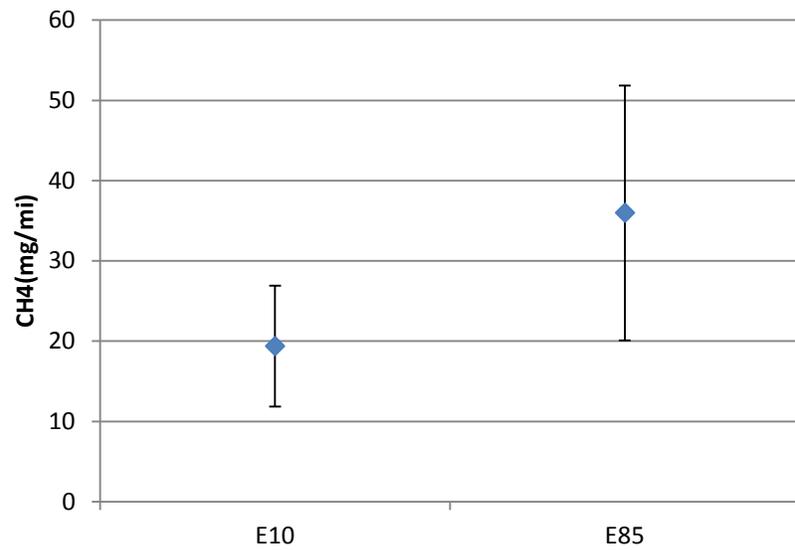


Figure 7-5. Mean NO_x Emissions from Vehicles Running on E10 and E85.

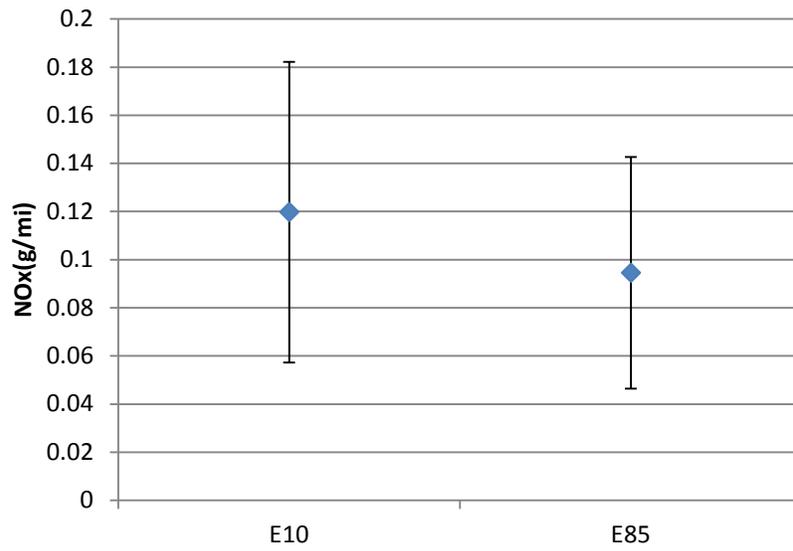


Figure 7-6. Mean PM_{2.5} Emissions from Vehicles Running on E10 and E85.

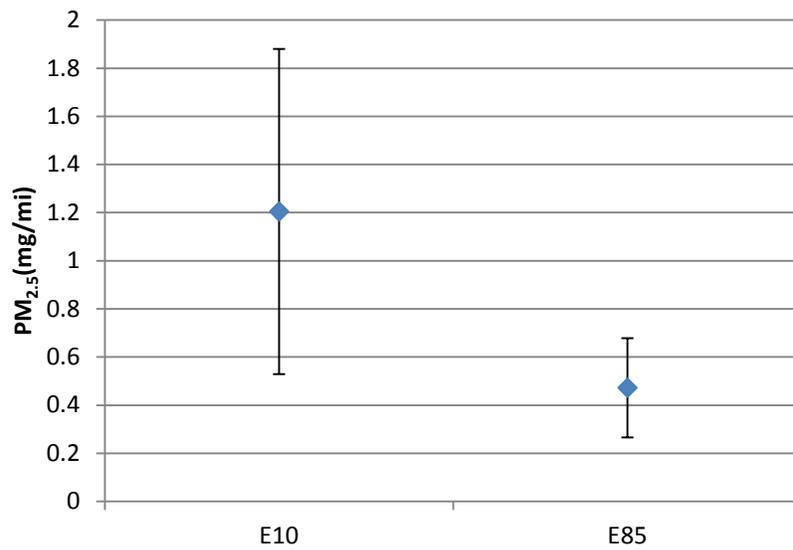
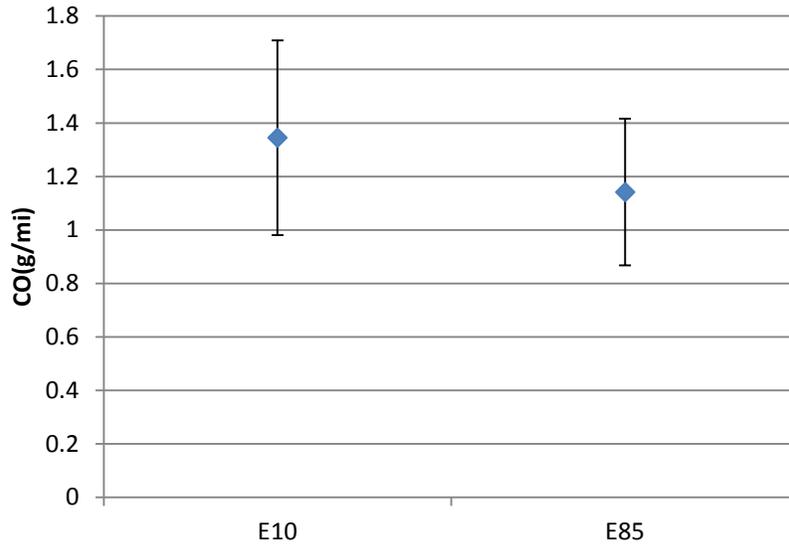


Figure 7-7. Mean CO Emissions from Vehicles Running on E10 and E85.



Although the 95% confidence intervals of the mean overlapped between E10 and E85 for all pollutants, to assess whether their population means differ statistically, the tests of significance between E10 and E85 were performed using Student’s paired *t*-tests for the pooled dataset.

As shown in Table 7-7, the emissions for E10 and E85 did not result in statistically significant differences for THC, NMOG, and NO_x. For PM_{2.5}, although a couple of vehicles showed reduction in emission between E10 and E85, the paired *t*-test showed no statically significant difference. The difference in CO emissions was nearly statistically significant. Only NMHC and CH₄ emissions showed statistically significant differences between E10 and E85.

Table 7-7. Tests of Significance using Student’s Paired T-Tests.

Pollutant	<i>p</i> -value
THC	0.7968
NMOG	0.3056
NMHC	0.0046
CH ₄	0.0226
NO _x	0.1667
PM _{2.5}	0.2797
CO	0.0665

7.3 Application in MOVES

Based on the analysis in Section 7.2, the gasoline rates for THC, CO, NO_x and PM_{2.5} are replicated for high-level ethanol blends (E85) in the database table, emissionRateByAge, for vehicles allowed to use E85 – passenger cars, passenger trucks, and light commercial trucks.

Similarly, the fuel effect adjustments for E10, including the effect of fuel sulfur, are applied to E85 in the *generalFuelRatioExpression* table, described in Section 6.5 (page 87).

In MOVES, the estimation of the other hydrocarbon emissions starts with THC. MOVES calculates both methane and NMHC from THC emissions using methane/total hydrocarbon ratios (CH4THCRatio in the database table *methaneTHCRatio*). Consistent with the results, FFVs fueled with E85 are projected to produce higher methane emissions than E10 and therefore, correspondingly lower levels of NMHC compared to E10. The development of the methane/total hydrocarbon ratios for E85 is documented in the MOVES2014 Greenhouse Gas and Energy Consumption Rates Report.⁶¹

For calculation of NMOG emissions for model year 2001 and later FFVs using E85, the exhaust speciation factors for E10 were used, because no statistically significant difference was observed between E10 and E85. Although volatile organic compounds (VOC) were not analyzed, due to a lack of speciated data, it was assumed that VOC would behave similarly to NMOG in terms of response to high-level ethanol blends for model year 2001 and later FFVs, since the only differences between NMOG and VOC are the presence of ethane and acetone. Therefore, the VOC/NMHC ratios used for E10 are also used for FFVs fueled with E85. For a detailed description of the algorithm used to estimate NMOG and VOC emissions from E85, see Appendix D of the MOVES2014a software design reference manual.⁶²

8 Biodiesel Blends

MOVES contains two fuel effects for diesel, based on the sulfur and biodiesel content of the fuel. For diesel vehicles, MOVES has fuel sulfur effects for particulate sulfate and gaseous sulfur dioxide emissions as described in Chapter 9 below. Unlike gasoline, no relationships between sulfur and HC, CO, and NO_x emissions are estimated in MOVES for diesel vehicles.

MOVES contains biodiesel effects that are applied to HC, CO, NO_x and PM. The biodiesel effects also affect the speciated hydrocarbon and particulate species that are derived from HC and PM emissions, even though the same toxic fractions (e.g. benzene/VOC) are applied to estimate toxic emissions from conventional diesel and biodiesel fueled vehicles.⁶³

As for sulfur, separate effects are modeled for pre-2007 and post-2007 technology diesel engines.

8.1 *Pre-2007 Diesel Engines*

The biodiesel effects implemented in MOVES are obtained from an analysis conducted in the course of the 2010 Renewable Fuel Standard Program.⁶⁴ The biodiesel effects were derived from an analysis of publicly available datasets on the effect of biodiesel on emissions from medium-duty and heavy-duty diesel engines that are representative of the in-use US fleet. The effect of a blend containing 20% biodiesel (B20) derived from this study is presented in Table 8-1. Additional analysis and discussion of the results are contained in EPA (2010).

Table 8-1. Emission impacts for all cycles tested on 20 vol% soybean-based biodiesel fuel relative to an average base fuel. (Reproduced from Table ES-A from the EPA (2010⁶⁴))

Pollutant Name	Percent Change in Emissions
HC	-14.1%
CO	-13.8%
NO _x	+2.2%
PM _{2.5}	-15.6%

This analysis evaluated only the impact of B20 on diesel emissions. The study did not evaluate the impact on gaseous emissions beyond the 20% biodiesel volumes.

8.2 *2007 and later Diesel Engines*

The analysis conducted by the Renewable Fuel Standard did not include 2007+ diesel engines or associated emission control technologies (including diesel particulate filters and selective catalytic reduction). Consistent and significant biodiesel effects have not been observed for 2007+ engines.^{65,66}

8.3 Modeling Biodiesel

The fuelFormulation table contains a parameter, “*bioDieselEsterVolume*,” that represents the volume percentage of biodiesel ester in a target fuel. The default fuel supply contains estimates of biodiesel volumes for fuel regions in the United States, as described in the fuel supply report. However, users can also enter local information about biodiesel fuels.

Mathematically, the *bioDieselEsterVolume* is used with a set of “biodiesel factors” (presented in Table 8-2). For pre-2007 engines, these factors are designed to give the fractional changes shown in Table 8-1, for a *bioDieselEsterVolume* of 20 vol.%. For volumes less than 20 vol.%, the fractional change is linearly interpolated between 0% and the change at 20 vol.%; for volumes greater than 20 vol.%, the fractional change for 20 vol.% is applied. In combination, these two parameters produce an overall fuel adjustment for biodiesel fuels.

Table 8-2 Biodiesel Fuel Adjustment Factors

Pollutant Name	BioDiesel Factor	
	Pre-2007 Diesel	2007+ Diesel
HC	-0.705	0
CO	-0.690	0
NO _x	0.110	0
PM2.5	-0.780	0

These fuel adjustments give the relative change in emissions associated with adding biodiesel to petroleum diesel fuel. The formulation for the fuel adjustment is shown in Equation 8-1.

$$\text{Fuel Adjustment} = 1 + \frac{\text{least}(\text{bioDieselEsterVolume}, 20)}{100} \times \text{bioDieselFactor} \quad \text{Equation 8-1}$$

To estimate adjusted emissions, the fuel adjustment is multiplied to the base emissions estimate, which represents operation on petroleum diesel. Note that currently there are no diesel fuels with biodiesel levels above 20 vol.% in the MOVES2014 default fuel supply. For 2007+ and later diesel, the biodiesel fuel adjustment factor is set equal to 0, consistent with the literature review in Section 8.2.

9 Sulfate Emissions

9.1 Introduction

Sulfate (SO_4) is an important contributor to primary exhaust particulate matter emissions from motor vehicles. The formation of sulfate from motor vehicles is a function of the engine combustion, emission control technology conditions, and the sulfur content in the fuel and the lubricating oil. MOVES2010b assumed that all sulfate emissions originated from the fuel sulfur, and based the sulfate calculations entirely from fuel consumption. Research on current technology diesel engines run on ultra-low sulfur diesel has shown that the sulfur contribution of lubricating oil can be more important than that of fuel in forming sulfate emissions.⁶⁷ For diesel engines equipped with catalyzed diesel particulate filters, the sulfate contribution from lubricating oil can also make up a substantial fraction of the $\text{PM}_{2.5}$ exhaust emissions.⁶⁸

Maintaining the capability to model high fuel-sulfur levels is important for MOVES. The particulate emission rates used in MOVES for gasoline and pre-2007 diesel were derived from sets of measurements on higher fuel-sulfur levels; it is thus important that MOVES be able to account for changes in fuel sulfur content in estimating particulate emissions. In addition, MOVES is used by international users, in regions where fuel sulfur levels can be much higher than current US levels.

MOVES2014 includes two major changes to improve the modeling of sulfate emissions. First, sulfate emissions are estimated from $\text{PM}_{2.5}$ emissions rather than from fuel consumption. This approach assures that the reference fraction of sulfate is consistent with the $\text{PM}_{2.5}$ emissions profile. Second, MOVES2014 accounts for sulfate contributions from both the lubricating oil and the fuel. Using particulate matter test programs conducted by the US EPA and reported in the literature, the relative contribution of sulfate emissions from lubricating oil and fuel is estimated.

This chapter includes an overview of the MOVES2014 sulfate calculator, and analysis conducted to determine the necessary inputs for 1) gasoline engines, 2) conventional diesel engines, 3) 2007 technology diesel engines, and 4) compressed-natural-gas engines. Additionally, the MOVES2014 algorithm for estimating sulfur dioxides is included in this chapter for consistency. The algorithm for gaseous sulfur-dioxide (SO_2) emissions remains the same as in MOVES2010b and is based on fuel consumption, but the parameters have been updated in MOVES2014 to be consistent with the changes to the sulfate emission factors.

9.2 Sulfate Calculator Summary

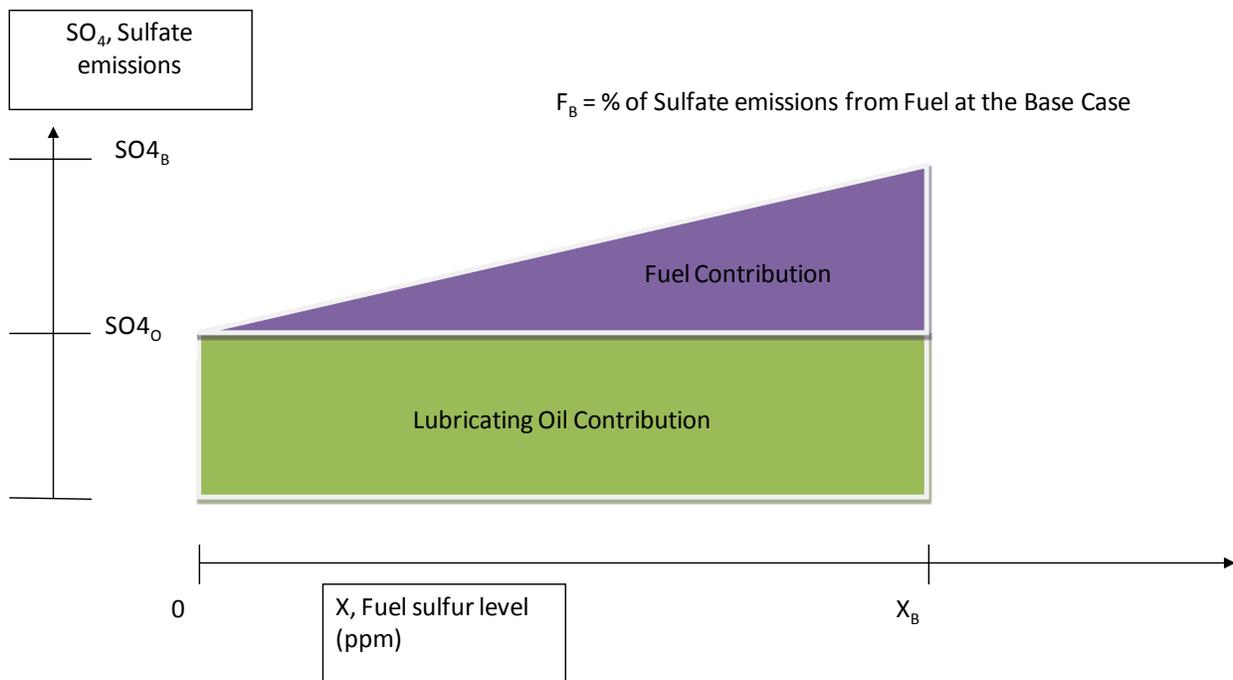
The MOVES2014 sulfate calculator adjusts the reference sulfate emissions using the following assumptions:

1. Sulfate emissions from the lubricating oil are constant regardless of the fuel sulfur level.
2. Sulfate emissions originating from the fuel scale linearly with changes in fuel sulfur level.

These assumptions are illustrated in Figure 9-1. Research on sulfur levels in lubricating oil and diesel fuel support these assumptions. Allansoon et al.⁶⁹ and Kittelson et al.⁶⁷ treated the sulfate contribution from the lubricating oil independently of the fuel sulfur level from diesel engines.

Wall et al.⁷⁰ demonstrated that sulfate emissions from diesel engines decrease linearly with decreases in the diesel fuel sulfur level down to 100 ppm and 0 ppm. Baranescu⁷¹ and Hochhauser⁷² affirmed that changes in diesel fuel sulfur did not affect the sulfur to sulfate conversion rate from conventional diesel engines operating on different driving cycles. Kittelson et al.⁶⁷ also assumed a constant relationship between fuel sulfur level and particle number emissions from modern trap-equipped diesel engines.

Figure 9-1. Schematic of Fuel and Lubricating Oil Contributions in MOVES2014.



The sulfate calculator uses the concept of reference emission rates and sulfate fractions. MOVES2014 adjusts the sulfate emissions based on differences between the sulfur content of the reference test program, and the user-supplied fuel sulfur content in a MOVES run. In MOVES2014, the base PM_{2.5} rates are divided between elemental carbon (EC) and the remaining PM that is not elemental carbon (NonECPM). MOVES2014 incorporates these modeling assumptions into Equation 9-1, the derivation of which is included in Appendix A:

$$SO4_x = NonECPM_B \times S_B \times \left[1 + F_B \times \left(\frac{x}{x_B} - 1 \right) \right] \quad \text{Equation 9-1}$$

where: $NonECPM_B$ is the reference non-elemental carbon PM_{2.5} emission rate, S_B = the reference sulfate fraction, x = the user-supplied or default fuel sulfur level for the MOVES run, x_B = the reference fuel sulfur level, and F_B = the percentage of sulfate originating from the fuel

sulfur in the reference case, and SO_{4x} = sulfate emissions at the fuel sulfur content for the MOVES run.

The S_B , F_B , and x_B , parameters vary by vehicle sourceType, model year group, and emission process as shown in Table 9-1. The only value that changes across moves runs, is the actual fuel sulfur level, x , which is either specified by the MOVES user, or is drawn from the MOVES2014 default fuel formulation and fuel supply table which specifies fuel properties and usage according to the geographic fuel region and calendar year. Each of the needed parameters for the sulfate calculator (S_B , F_B , x_B) are provided in Table 9-1, which is stored in the MOVES table “*sulfateFractions*.” The sulfate calculator works in concert with other calculators in MOVES to estimate PM_{2.5} emissions. A flow chart which illustrates the context in which the sulfate calculator is involved in estimating PM_{2.5} emission rates is shown in the MOVES2014 Speciation report.⁷³

Sulfate-bound water (H₂O aerosol) is a new pollutant in MOVES2014. Currently, the value of H₂O_B in MOVES2014 is 0 for all on-road source types, as derived from the PM_{2.5} speciation profiles (cite Speciation report). If included in the PM_{2.5} speciation profile, the H₂O aerosol is assumed to be associated with sulfate, and is scaled using the same relationship with fuel sulfur level, as shown in equation:

$$(H_2O)_x = NonECPM_B \times (H_2O)_B \times \left[1 + F_B \times \left(\frac{x}{x_B} - 1 \right) \right] \quad \text{Equation 9-2}$$

where $(H_2O)_B$ is the fraction of water-bound sulfate in the *NonECPM*.

Table 9-1. Coefficients for the Sulfate Calculator in MOVES2014

Source	Process	Reference Fractions		Reference fuel sulfur Level, ppm (x_B)	Reference estimated fraction from fuel sulfur (F_B)
		SO ₄ /PM _{2.5}	SO ₄ /NonEC PM (S_B)		
Gasoline	running exhaust	7.2%	8.4%	161.2	68.7%
	start exhaust	0.9%	1.7%		
Pre-2007 diesel	running exhaust	1.0%	4.9%	172.0	72.6%
	start, extended idle and apu	5.3%	9.8%		
2007+ diesel	running, extended idle, start	67.6%	73.6%	11.0	48.3%
Pre-2002, compressed natural gas	running, extended idle, start	0.6%	0.7%	5.0	0.0%
2002+ Compressed natural gas	running, extended idle, start	1.0%	1.2%	5.0	0.0%

The following section discusses the derivation of the parameters displayed in Table 9-1 for 1) gasoline vehicles, 2) conventional diesel vehicles, 3) 2007 technology diesel vehicles, and 4) compressed natural gas vehicles.

9.3 Gasoline Vehicles

The reference sulfate fractions and the reference fuel sulfur level for gasoline vehicles are estimated from the Kansas City Light-Duty Vehicle Emissions Study (KCVES). The use of the KCVES for estimating PM_{2.5} emission rates is documented in the MOVES2014 Light-duty Vehicle Emission Rate report,⁴⁸ and the derivation of the sulfate emission factor is documented in the MOVES 2014 TOG and PM Speciation Report.⁷³ The reference fuel sulfur content (161.2 ppm) was calculated using 171 fuel analysis samples from the KCVES. The high sulfur content of the fuels tested in KCVES is a limitation when applying the speciation profile to Tier 2 and Tier 3 gasoline. But as discussed in the Speciation report, the KCVES PM_{2.5} speciation profile is the most representative profile available to EPA at this time to represent PM emissions from in-use light-duty gasoline vehicles.

The reference contribution of fuel sulfur to the sulfate emissions (68.7%) is estimated from an analysis that combined data from the KCVES, which tested vehicles using high fuel-sulfur content, with light-duty gasoline vehicles tested at a low fuel-sulfur content (6 ppm) as part of the Full Useful Life (FUL) Test Program.⁷⁴ The FUL program was the most relevant study available to the US EPA that measured sulfate emissions from low-sulfur gasoline available that could be used to evaluate the impact of low-sulfur gasoline fuel on light-duty engines. By using the FUL test program in the analysis, the sulfate fraction estimated by MOVES is based on actual data tested on Tier 2 vehicles on low-sulfur fuels. An overview of the data and the analysis performed to calculate the reference contribution of fuel sulfur to sulfate emissions is provided in Appendix A.

The sulfate values derived in Table 9-1 are used for all gasoline sourceTypes in MOVES, including motorcycles, light-duty passenger-cars and trucks, medium-duty and heavy-duty gasoline trucks, and gasoline-powered buses. Applicable sourceType identifiers include 11, 21, 31, 32, 42, 43, 52, 53, 54, and 61.

9.4 Pre-2007 Diesel Vehicles

The reference sulfate fraction of PM_{2.5} is derived from the Heavy-Duty Vehicle Chassis Dynamometer Testing for Emissions Inventory, Air Quality Modeling, Source Apportionment and Air Toxics Emissions Inventory (E55/59).⁷⁵ The E55/59 study is also used to derive the PM_{2.5} emission rates for medium and heavy-duty diesel in MOVES2014 (MOVES2014 heavy-duty report). The estimated fuel sulfur content of diesel trucks tested in E55/59 is 172 ppm, based on in-tank fuel samples from three vehicles in the program that were selected for standard fuel analysis^c.

To estimate the relative contribution of lubricating oil and fuel from conventional diesel engines, data collected from the Diesel Emissions-Control Sulfur Effects Project (DECSE) was used.⁷⁶ The DECSE project was conducted to investigate the impact of low-sulfur diesel fuel standards

^c See Table 11 in Clark et al.⁷⁵

on diesel emissions. Specifically, the DESCE conducted testing of two engines at four sulfur levels: 3, 30, 150, and 350 ppm. Sulfate emissions were measured at each of the levels. These data were used to calculate the 72.6% contribution of the fuel to sulfate emissions at the reference fuel-sulfur level (172 ppm) for the base pre-2007 diesel rates in MOVES2014. The sulfate emissions estimated from the fuel-sulfur (72.6%) are then scaled linearly with changes in fuel-sulfur relative to the reference fuel sulfur level (172 ppm) using Equation 9-1. Details on the analysis used to derive the relative fuel contribution to pre-2007 diesel sulfate emissions from the DESCE data are provided in the appendix.

9.5 *2007 and Later Technology Diesel Vehicles*

The sulfate contribution of the fuel and lubricating oil for 2007 and later diesel vehicles is based on a study designed and conducted by Kittelson et al.⁶⁷ The study evaluated the contribution of lubricating oil and diesel fuel to ultrafine particle emissions from a modern diesel engine equipped with a catalyzed diesel-particulate filter (C-DPF). The researchers estimated a linear model that predicts the ultrafine particle-number emissions from the sulfur content in the lubricating oil and the fuel. We adapted this analysis by assuming that the relative contribution of lubricating oil and fuel to sulfate emissions is the same as their relative contribution to the ultrafine particle emissions. We applied the coefficients developed by Kittelson et al. to estimate the relative contributions of lubricating oil and fuel to sulfate emissions at fuel-sulfur levels in fuel and lubricating oil of 11 ppm and 3,000 ppm. Eleven ppm is selected as the reference fuel-sulfur content used in MOVES2014. The sulfur level in oil (3,000 ppm) is the sulfur content assumed by Kittelson et al. for trap-equipped diesel engines, lower than 4,000 ppm limit specified by API category CJ-4 lubricating oil used for 2006 and later diesel engines.⁷⁷ Using these assumptions, the lubricating oil is estimated to contribute the majority of the sulfate emissions (51.7%) when the fuel-sulfur is 11 ppm.

The reference sulfate fraction is based on the PM_{2.5} speciation profile for 2007 and newer on-highway diesel technology, based on Phase 1 of the Advanced Collaborative Emissions Study (ACES).⁷⁸ The Phase 1 study tested four heavy-duty diesel engines, each equipped with a catalyzed diesel-particulate filter (C-DPF), over a 16-hour cycle specifically developed for this purpose. The PM_{2.5} speciation profile for 2007 and later diesel engines used in MOVES2014 is based on data acquired from these four engines. The fuel-sulfur level tested in the ACES program is 4.5 ppm.⁶⁷ The sulfate fraction from the ACES Phase 1 project is adjusted to account for a level of 11 ppm assumed to apply to base PM_{2.5} emission rates for engines manufactured in 2007 and later. Using Equation 9-1 and the derived parameters in Table 9-1 a SO₄/PM_{2.5} fraction for 11 ppm fuel is estimated to be 67.6% (as compared to 59.1% at 4.5 ppm). This fraction is used as the reference sulfate fraction for 2007 and later diesels in MOVES2014 as shown in Table 9-1. Additional details on the analysis are included in Appendix A.4.

9.6 *Compressed Natural Gas*

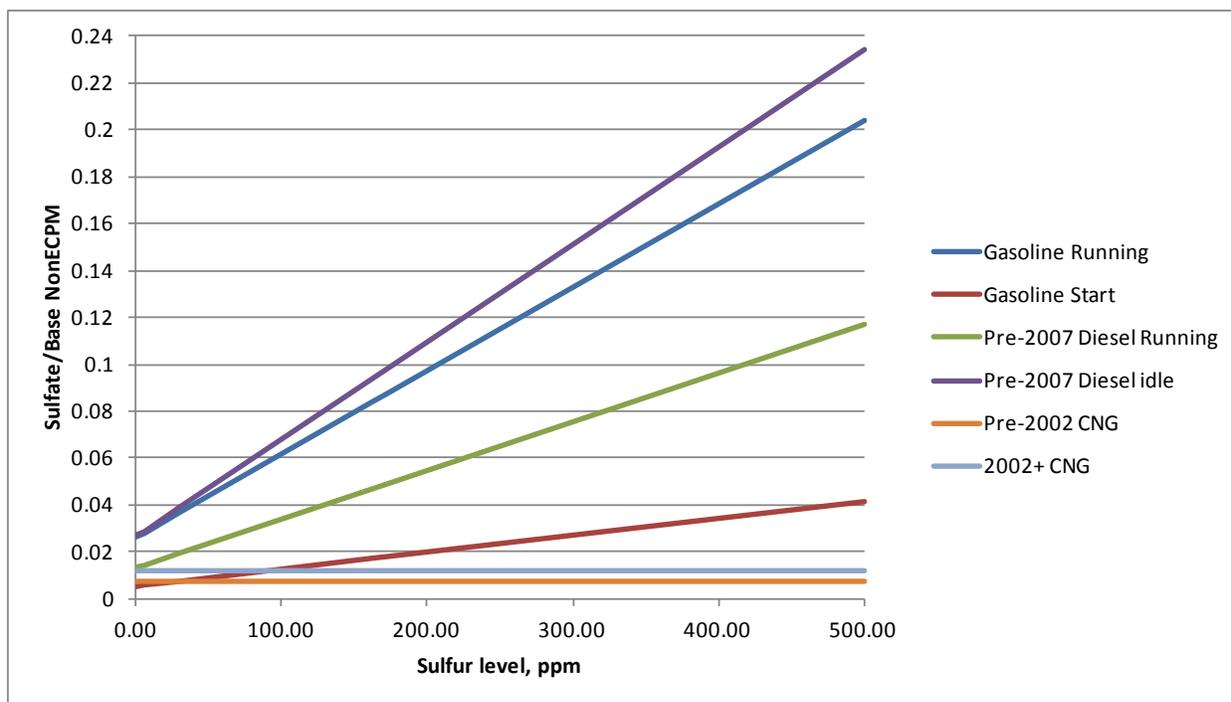
We had limited data on sulfate emissions from engines running on compressed natural gas, especially regarding the relative contribution of the lubricating oil and CNG fuel to sulfate emissions. As such, we do not adjust the sulfate emissions according to fuel sulfur level. We derived a constant fraction of sulfate emissions from elemental sulfur emissions measured by the California Air Resources Board on a CNG transit bus with a 2000 MY Detroit Diesel Series 50

engine with and without an oxidation catalyst as documented in the MOVES Speciation Report.⁷³ We set F_B coefficient to 0, so that MOVES estimates the same sulfate emissions regardless of the sulfur level in the CNG fuel.

9.7 Example Comparisons

Figure 9-2 plots the sulfate/nonECPM ratios calculated from the parameters in Table 9-1 across a range of sulfur levels from 0 to 500 ppm. We excluded the 2007+ diesel values from this plot, because those vehicles have much higher sulfate PM fractions, and 2007+ diesel vehicles operate only on ultra-low-sulfur diesel (sulfur concentration < 15 ppm). This figure demonstrates that sulfate levels can range from less than 4% of NonECPM at low sulfur levels, to over 20% of NonECPM at high fuel-sulfur levels.

Figure 9-2. Sulfate/Base nonECPM emission rates calculated from Equation 9-1 and the parameters in Table 9-1 across a range of fuel sulfur levels.



In Figure 9-3, we show estimated SO_4 mass emission rates by combining the estimates in Figure 9-2 with estimates of NonECPM emission rates from gasoline passenger cars, heavy-duty diesel long-haul combination trucks, and CNG transit bus emissions estimated using MOVES2014 for a state-wide (Michigan) run in calendar year 2011.

The base NonECPM emission rates in MOVES2014 for pre-2007 diesels are based on a reference sulfur level of 172 ppm (Section 9.4). At this level, the sulfate emission rate across all processes is ~ 20 mg/mile [12 mg/mile (running) + 8 mg/mile (idle/start)]. At 2007+ diesel sulfur levels (15 ppm), MOVES estimates sulfate emissions of ~ 7 mg/mile [4 mg (running) + 3 mg/mile (idle/start)]. For this MOVES scenario, the sulfate calculator in MOVES reduces sulfate

PM (and total PM_{2.5} emission rates) from the reference pre-2007 diesel PM emission rates by ~ 13 mg/mile.

Similarly, the reference sulfur level for gasoline vehicles in MOVES is 161.2 ppm (Section 9.3). Reducing the sulfur levels to Tier 3 gasoline sulfur levels (10 ppm), reduces the sulfate emissions by approximately 1 mg/mile, from 1.2 mg/mile to 0.4 mg/mile.

Figure 9-3. Example SO₄ emission rates as a function of fuel sulfur level (0 to 500 ppm) estimated from a MOVES2014 for the state of Michigan, in calendar year 2011 run for Michigan using national default data.

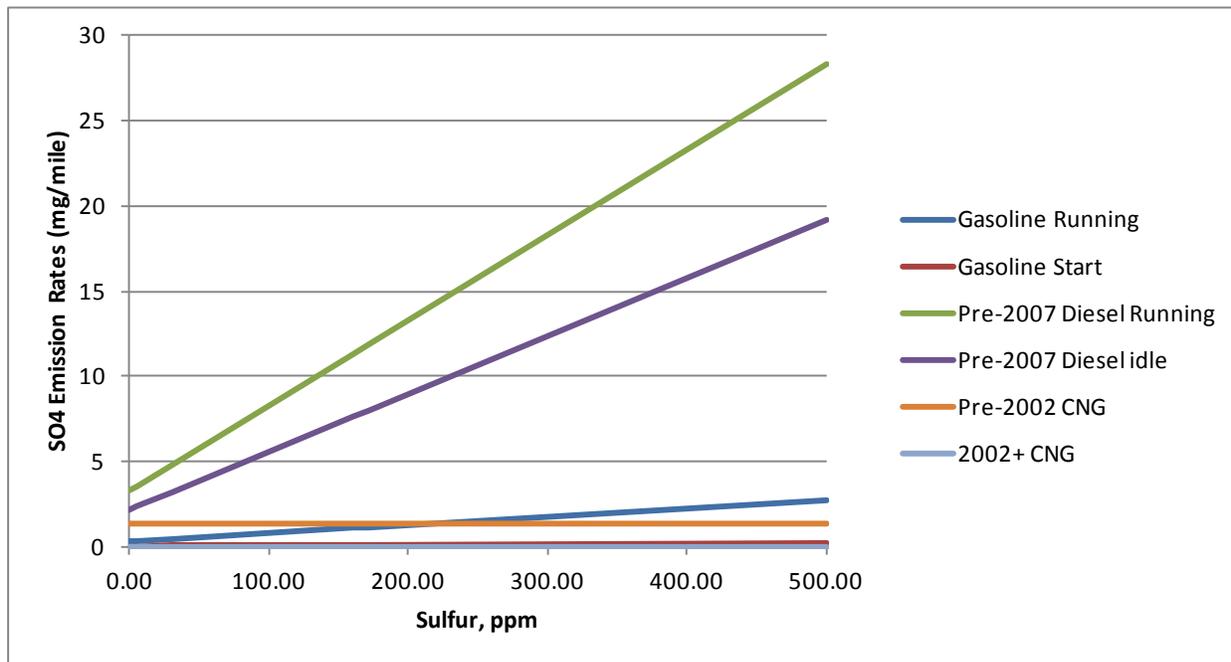
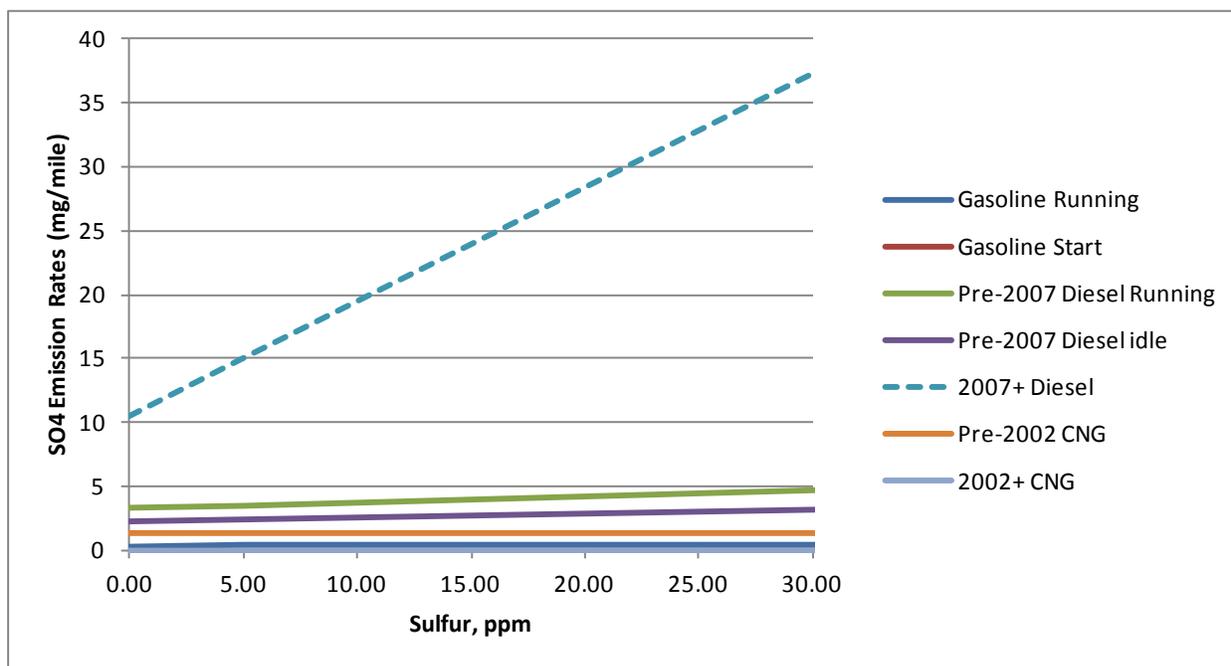


Figure 9-4 plots the estimated sulfate emissions (including 2007+ diesel engines) across a smaller range of fuel sulfur levels (0 to 30 ppm). The 2007+ diesel engines clearly has the largest sulfate emission rates (mg/mile) across all sulfur levels, and also have the largest sensitivity to fuel sulfur levels. This is not surprising, because the 2007+ trucks have a large sulfate fraction in the reference rates, coupled with a low reference sulfur level (11 ppm). The 2007+ diesel engines are estimated to emit ~ 20 mg/mile sulfate at 11 ppm. This level is comparable to the estimated volume of sulfate emitted from the pre-2007 diesel trucks at 172 ppm.

The gasoline and pre-2007 diesel sulfate emission rates are relatively insensitive to sulfur changes within this range (0-30 ppm) of fuel sulfur content. The sulfate emissions from gasoline and pre-2007 diesel trucks contribute less than 4% of the NonECPPM emission rates (and less than 3% of total PM_{2.5} emission rates), and the contribution changes by only ~1% between 0 and 30 ppm.

Figure 9-4. Example SO₄ emission rates as a function of fuel sulfur level (0 to 30 ppm) estimated from a MOVES2014 for the state of Michigan, in calendar year 2011 run for Michigan using national default data.



Comparisons of the sulfate calculator to other reported values in the literature for gasoline and pre-2007 diesel are presented in Appendix A.

9.8 Sulfur Dioxide Emissions Calculator

The sulfur dioxide (SO₂) emissions algorithm is unchanged from MOVES2010b, but the parameters are updated to be consistent with the updated analysis on sulfate emissions. The MOVES SO₂ algorithm calculates SO₂ emissions using three parameters (1) total fuel consumption, (2) fuel sulfur level, and (3) the fraction (%) of fuel sulfur emitted as sulfate emissions.

Unlike the sulfate calculator, the SO₂ calculator assumes that all of the sulfur in SO₂ emissions originate from the fuel. This assumption is reasonable because on a mass-balance basis most of the sulfur originates from the fuel, even at low fuel-sulfur levels. The reason that sulfur in the lubricating oil has a large impact on sulfate emissions is that the sulfur in the lubricating oil has a much high propensity to form sulfate than sulfur burned in the fuel.⁶⁷

SO₂ emissions are calculated using Equation 9-3:

$$SO_2(g) = FC(g) \times [S] (ppm) \times \frac{MW_{SO_2}}{MW_S} \times fSO_2 \times \left(\frac{10^{-6}}{ppm} \right) \quad \text{Equation 9-3}$$

where

$FC(g)$ = fuel consumption (g), and

$[S]$ (*ppm*)= relative fuel-sulfur concentration (*ppm*)

$\frac{MW_{SO_2}}{MW_S}$ is the ratio of the molecular weight of sulfur dioxide as defined in Equation 9-4.

$$\frac{MW_{SO_2}}{MW_S} = \frac{32 + (2 \times 16) \frac{g}{mol}}{32 \frac{g}{mol}} = 2.0 \quad \text{Equation 9-4}$$

f_{SO_2} = Fraction of fuel sulfur that is converted to gaseous SO₂ emissions. The SO₂ conversion fraction is calculated as the fraction of fuel sulfur not converted to sulfate.

In MOVES2014, the SO₂ calculator first calculates the product of $FC(g) \times [S]$ (*ppm*). Then it multiplies the product by the SO₂ emission factor which combines the last three terms of Equation 9-3 including the ratio of molecular masses Equation 9-4.

The SO₂ conversion values and resulting SO₂ emission factors for use in MOVES2014 are displayed in Table 9-2.

Table 9-2. SO₂ conversion efficiencies and MOVES SO₂ emission factors.

Source	SO ₂ conversion efficiency (%)	SO ₂ EF (1/ppm)
Gasoline	99.69%	1.994E-06
Pre-2007 Diesel	94.87%	1.897E-06
2007 Diesel	88.15%	1.763E-06
CNG	100%	2.000E-06

The SO₂ conversion factors for gasoline are based on the VMT-weighted values from the Kansas City study. The updated SO₂ conversion values (99.69%) for gasoline engines are slightly lower than the previous values used in MOVES2010b (99.84%), which is required to provide consistent rates with the updated sulfate emission rates. These values are used for all highway gasoline sources.

Fuel consumption data were not available from the E55/59 study which was used as the source of the sulfate emission rates for diesel engines. The updated SO₂ conversion values for the pre-2007 diesel were calculated by achieving sulfur balance with the estimated fuel sulfur consumed and sulfate emissions from pre-2007 diesel trucks, with both quantities estimated using MOVES. A 2014 national MOVES inventory was calculated for pre-2007 single and combination diesel trucks, with the fuel sulfur assigned to a level derived from the E55/59 study (172 ppm). The sulfate speciation factor and percentage of sulfate coming from the fuel were taken from Table 9-1. The analysis estimated that 5.13% of the fuel sulfur forms sulfate emissions, leaving an estimated SO₂ conversion value of 94.87%. MOVES2010 assumed that 2% of fuel sulfur formed sulfate emissions, which was taken from the US EPA PART5 model used in previous versions of MOVES and MOBILE (EPA, 2003). MOVES2014 thus assumes a larger percentage of fuel sulfur forms sulfate emissions in conventional diesel engines. The 2007 diesel SO₂ emissions

factor is based on calculations using the reported fuel consumption and sulfate emissions from the ACES Phase 1 report, along with the data from the sulfate calculator for sulfate emissions. The SO₂ conversion factor for 2007 and later diesel (88.15%) is considerably larger than the SO₂ assumed in MOVES2010b (54.16%). The reason for the large shift is the large contribution of lubricating oil to sulfate emissions accounted for in MOVES2014. The diesel values are used for all on-highway diesel sources for 2007 and later.

In the absence of other data, we assume that 100% of the sulfur in the CNG fuel forms SO₂ emissions. This is a reasonable simplification because the sulfur content of CNG is low in comparison to diesel and gasoline, and because lubricating oil also contributes to SO₂ emissions. This assumption is also consistent with our assumption for the formation of sulfate emissions from CNG engines. Lanni et al.⁷⁹ measured SO₂ and SO₄ emissions from three CNG transit buses. The sulfur content of the CNG fuel was not reported, but by assuming that all of the fuel sulfur is converted to SO₂ emissions we estimated a CNG sulfur content of 7.6 ppm. Ayala et al.⁸⁰ reported that the maximum allowable fuel sulfur content for use in CNG motor vehicles is 16 ppmv. The Energy Information Administration reports that the fuel sulfur content of natural gas at the burner tip is less than 5 ppm.⁸¹ For use in MOVES, we selected the default sulfur level of CNG to be 7.6 ppm, to be consistent with the sulfur dioxide measurements conducted by Lanni et al.⁷⁹

9.9 Summary

The sulfate calculator is used to adjust sulfate (and thus the total PM_{2.5} emission rates) for gasoline and pre-2007 diesel trucks across a wide range of sulfur values. The reference sulfate emission rates for gasoline and pre-2007 diesel are based on reference fuel sulfur levels of 161 and 172 ppm, respectively. Current regulations require diesel sulfur levels to be less than 15 ppm, and gasoline less than 30 ppm, with further reduction in gasoline sulfur to 10 ppm required by 2017. When modeling these lower fuel sulfur levels, MOVES reduces the reference sulfate emission rates by ~ 10 mg/mile for pre-2007 diesel trucks, and ~ 1 mg/mile for gasoline cars.

While the sulfate calculator is important to adjust the pre-2007 diesel and gasoline emission rates for large fuel sulfur changes, the sulfate calculator has a minimal impact on the sulfate emissions for small sulfur changes (e.g. less than 30 ppm changes), which reflect the large contribution of lubricating oil to sulfate emissions at low fuel sulfur levels. In contrast, sulfate emissions from 2007+ diesel technology engines are highly sensitive to the fuel sulfur level, because these engines produce a high amount of sulfates even at very low fuel sulfur levels.

Because PM_{2.5} and sulfate emissions are relatively low from CNG vehicles, we maintained a simple sulfate emission rates in MOVES for these vehicle types that do not adjust the sulfate emissions to the sulfur-content of the CNG fuel.

We also updated the values in the MOVES SO₂ calculator, such that the SO₂ and sulfate emissions approximately achieve a mass balance with the sulfur consumed in the fuel.

Additionally work is needed to quantify the sulfate emissions from advanced engine and emission control technologies in MOVES, including: 2010 DPF/selective-reduction-catalyst equipped diesel engines, light-duty diesel engines, lean-burn gasoline, and direct injection gasoline vehicles. Because the inputs to the sulfate calculator are table-driven, these values can be updated as new data become available.

Appendix A Derivation of the Sulfate Equation and Parameters

A.1 Derivation of Calculations Performed in the Sulfate Calculator

The following equation is used to model the Sulfate emissions:

$$SO4_x = (\text{Sulfate from oil}) + (\text{Sulfate from Fuel}) \quad \text{Equation A-1}$$

$$SO4_x = NonECPM \times \left(S_B \left(\frac{S_O}{S_B} \right) + (S_B - S_O) \left(\frac{x}{x_B} \right) \right)$$

Where: $SO4_x$ = Sulfate level at fuel sulfur x , S_O = Fraction of sulfate emissions from lubricating oil, S_B = Sulfate fraction in the reference case, x_B = fuel sulfur level in the reference case.

Let F_B = % of sulfate from the fuel sulfur in the baseline case:

$$F_B = \frac{(S_B - S_O)}{S_B} \quad \text{Equation A-2}$$

Substituting Equation A-2 into Equation A-1 yields Equation A-3:

$$\begin{aligned} SO4_x &= NonECPM \times \left(S_B \times (1 - F_B) + S_B \times F_B \times \left(\frac{x}{x_B} \right) \right) \\ &= NonECPM \times \left(S_B \times \left[1 - F_B + F_B \times \left(\frac{x}{x_B} \right) \right] \right) \\ &= NonECPM \times \left(S_B \times \left[1 + F_B \times \left(\frac{x}{x_B} - 1 \right) \right] \right) \end{aligned} \quad \text{Equation A-3}$$

Using Equation A-3 the sulfate emissions can be modeled, with the user supplied values of x (fuel sulfur level), and model parameters, S_B , F_B and x_B .

Similarly, the particulate water (H_2O) depends on the amount of sulfate in the exhaust, and thus the amount of fuel sulfur. The same adjustment to the sulfate-bound water will be applied to the reference water emission rate as shown in Equation A-4:

$$(H_2O)_x = NonECPM \times \left((H_2O)_B \times \left[1 + F_B \times \left(\frac{x}{x_B} - 1 \right) \right] \right) \quad \text{Equation A-4}$$

A.2 Derivation of the Sulfate Calculator Parameters for Light-duty Gasoline Vehicles

The KCVES collected PM_{2.5} measurements from a statistically representative sample of vehicles in the Kansas City Metropolitan Area. The study was conducted in the summer of 2004 (Phase 1) and winter of 2004/2005 (Phase 2). In total, 496 vehicles were measured over both phases of the program. Chemical speciation was estimated from a subset of 99 vehicles from the initial 496 vehicles. The vehicles were tested on the LA-92 cycle. The details of the KCVES are located in US EPA (2008⁸²) and Fulper et al. (2010⁸³).

A.2.1 Fuel Sulfur Content

The first step is to determine the sulfur content for the Kansas City vehicles from which the reference sulfate emission rates are derived. Analysis of the fuel properties was conducted on a subset of vehicles in KCVES. One hundred seventy-one vehicle tests in the KCVES were matched with a fuel analysis reported in the Kansas City PM Characterization Report^d. The average fuel sulfur content is shown in Table 2-1, with associated 95% confidence intervals. The mean sulfur content is significantly lower in the summer, as shown by the 95% confidence intervals. Interestingly, the winter measurements had higher sulfur content, although they were closer to the phase-in of the Tier 2 low-sulfur standards.

Table A-1. Mean Fuel Sulfur content by Season.

Season	n	Mean sulfur content, ppm	sd	95% Lower Confidence level	95% Upper Confidence level
summer	98	138.8	83.0	122.1	155.4
winter	73	183.6	87.4	163.2	204.0

Because most of the vehicles that had a chemical analysis of the emissions did not have the fuel analysis conducted, the average fuel sulfur content from all the tests is used to represent the reference case fuel sulfur level. An equally weighted average of the summer and winter is used of 161.2 ppm.

^d The fuel sulfur content from 87 vehicles is reported in Tables 4-11 and 4-15 from the KC PM Characterization Report⁸². An additional 84 fuel samples were transcribed from the fuel analysis reports in Appendix ff, because the tests were not complete by the release of the initial report.

A.2.2 Fuel Sulfur Contribution Analysis

The sulfate-adjustments in MOVES 2014 consider the sulfate contribution from both the fuel and the lubricating oil. The following equation (A-4) is used to estimate the fuel and lubricating oil contribution for the gasoline engines:

$$\beta_1 \cdot OSE + \beta_2 \cdot FSC = SES \quad \text{Equation A-4}$$

Where: β_1 = Fraction of oil sulfur converted to sulfate, OSE = Oil-sulfur emissions in mg/mi, β_2 = Fraction of fuel sulfur converted to sulfate, FSC = fuel-sulfur consumption in mg/mi, SES = Sulfur- emitted as sulfate (mg/mi). SES is 1/3 the value of the sulfate emission rate, to only account for the mass of sulfur in the sulfate molecule (SO_4). To estimate parameters in Equation A requires at least two data points, ideally one data point at a high fuel sulfur level, and another at a low fuel sulfur level.

We used the KCVES as our data source from gasoline testing at a high fuel sulfur level. And we used a recent gasoline test program, the Full Useful Life (FUL) Test Program conducted at the National Vehicle Fuels & Emissions Laboratory in 2011 as our test program on low fuel sulfur. The Full Useful Life (FUL) Test Program conducted at the National Vehicle Fuels & Emissions Laboratory in 2011 evaluated light-duty gasoline Tier-2 vehicles (model year 2005 – 2009 vehicles) at ~ 120,000 miles. The FUL vehicles were tested at low fuel sulfur content (6 ppm), and sulfate measurements are made from the samples, on cold UDDS (bag 1 + bag 2 of the FTP), hot UDDS cycles, and hot US06 cycles. Documentation of the FUL test program is located in Sobotowski (2013).⁷⁴

Unfortunately, different vehicles were tested between the two studies. To best match the vehicle technologies and testing conditions, we only used the emissions data collected from the 1996-2004 vehicles in the KCVES, and only used the summer round data. Because the fuel sulfur content was not measured for each of the KCVES vehicles, we assumed that the fuel sulfur content is the mean fuel sulfur level measured in the summer (138.8 ppm). Comparisons of the particulate measurements of the elements are compared for the newest vehicles from Kansas City LA-92 cycle, with the three cycles measured in the FUL program in Figure A-1.

Figure A-1. Oil-derived metals (calcium, molybdenum, phosphorous, zinc), and sulfate and sulfur emission rates from the Full Useful Life Program, and the newest vehicles from the Kansas City study (1996-2004).

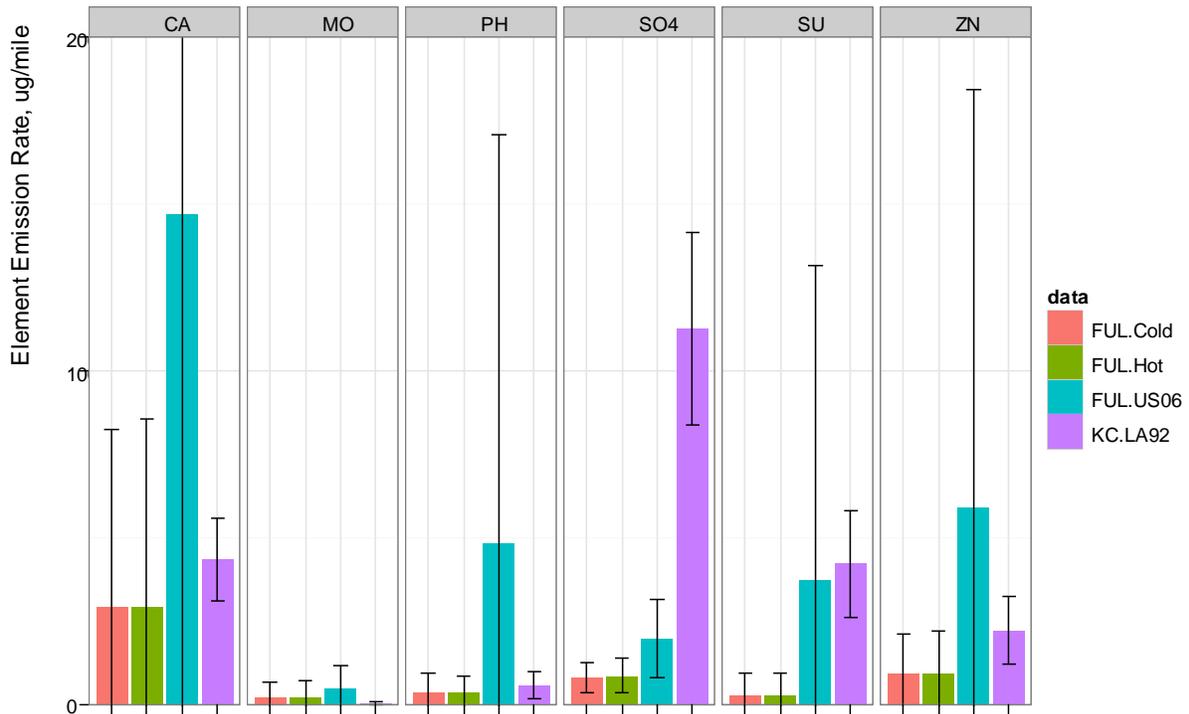


Figure A-1 contains the oil-derived metals (calcium, molybdenum, phosphorous, zinc), sulfate and sulfur emission rates from the Full Useful Life Program, from the newest vehicles from the Kansas City study (1996-2004) that are tested in the summer round. Calcium is the dominant element emitted in the exhaust, as well as the dominant metal component of lubricating oil. As shown, the calcium emissions on the FUL UDDS tests are comparable to the calcium emissions on the Kansas City LA-92 tests. The calcium emission rates from KCVES are slightly higher, which would be expected due to the slightly more aggressive LA-92 cycle compared to the FTP. In contrast, the US06 has very high oil element emissions in the FUL which is a very aggressive cycle, which could lead to high oil consumption/and or burn-off of particles on the catalyst and exhaust system. Overall, the oil consumption based on the element emission rates, appears to be comparable between the FUL and newest KCVES vehicles. The KCVES vehicles have much higher sulfate emission rates, which is expected due to the higher sulfur content in the fuel.

The two data sets (FUL vehicles, and the newest vehicles from KCVES) were combined to estimate the relative contribution of sulfate from the lubricating oil and the fuel. In combining the data sets, the 4 gasoline-direct injected vehicles are excluded from the FUL program to provide a comparison of port-fuel injection technology. Also the composite FTP values were used from the FUL test program ($0.43 \cdot \text{Cold UDDS} + 0.57 \cdot \text{Hot UDDS}$). Only the KCVES vehicles tested in the summer are included to minimize any confounding effects of temperature on sulfate and oil emissions. The following assumptions regarding the two sets of vehicles are made to estimate the sulfate contributions:

1. Sulfur that is consumed with the lubricating oil in the engine forms sulfate emissions with the same propensity between the FUL and KCVES vehicles. Oil consumption is not measured on the vehicles over each cycle. The sulfur emitted in the oil is estimated using the measured calcium emission rates, and the average sulfur to calcium concentration measured in the lubricating oil from the FUL test program. The ratio between calcium to sulfur concentration in the lubricating oil is assumed to be equal between the 1996-2004 KCVES vehicles and the FUL program vehicles.
2. The fraction of fuel sulfur converted to sulfate is the same between the FUL and 1996-2004 Kansas City vehicles. Both set of vehicles have port-fuel injected, closed looped engines with three-way catalysts emission control technologies.

The mean values from the KCVES (1996-2004) and the FUL vehicles are used to estimate the parameters in Table A-2. Weighted means were calculating, using the distribution of the cars and trucks from the KCVES for the 1996-2004 model years (57% cars, 43% light-duty trucks). The following data were used with Equation A:

For Kansas City:
$$\beta_1 \cdot \overline{OSE}_{KC} + \beta_2 \cdot \overline{FSC}_{KC} = \overline{SES}_{KC}$$

For the Full Useful Life Program:
$$\beta_1 \cdot \overline{OSE}_{FUL} + \beta_2 \cdot \overline{FSC}_{FUL} = \overline{SES}_{FUL}$$

Assumption 1 implies $\beta_1 = \beta_1$, and assumption 2 implies $\beta_2 = \beta_2$. With two unknowns, and two equations, β_1 and β_2 are estimated, and the model parameters are displayed in Table A-2. The fuel is estimated to contribute ~20% of the sulfate emissions for the FUL program vehicles, and over 70% of the sulfate emissions for the Kansas City vehicles.

Table A-2. Data, estimated coefficients, and estimated contributions of sulfate from the lubricating oil and fuel from the FUL and Kansas City studies.

Parameter	FUL (FTP)	Kansas City (LA-92)	Kansas City (LA-92)
Vehicle Model Year Range	2005-2009	1996-2004 (Summer only)	1968-2004 (VMT weighted)
Sulfur, ppm (x_B)	6	138.8	161.2
Calcium emissions, mg/mi	0.028	0.067	0.089
Sulfur/Calcium lubricant concentration ratio	0.697	-	-
Estimated oil sulfur emission, mg/mi (OSE)	0.020	0.047	0.062
Estimated fuel sulfur consumption, mg/mi (FSC)	0.849	21.648	25.033
Sulfate emissions, mg/mi	0.024	0.163	0.340
Fraction of Oil Sulfur Converted to Sulfate Emissions (β_1)	0.333	0.333	0.575
Fraction of Fuel Sulfur Converted to Sulfate Emissions (β_2)	0.0018	0.0018	0.003
Sulfate conversion adjustment (α)	1	1	1.726
Oil Sulfate Contribution, mg/mi	0.020	0.047	0.106
Fuel Sulfate Contribution, mg/mi	0.005	0.117	0.233
Oil Sulfate Contribution %	81.1%	28.5%	31.3%
Fuel Sulfate Contribution % (F_B)	18.9%	71.5%	68.7%

The sulfate PM speciation factors needed for MOVES 2014 gasoline vehicles were based on a fleet-average of the both the summer and winter tests. The model parameters were adjusted to be applicable for the fleet of vehicles measured in Kansas City. As stated earlier, the winter tests had significantly higher sulfur contents in than the summer tests. For modeling the fleet sulfate contributions in MOVES2014, the fuel contribution to sulfate emissions was estimated from the mean fuel sulfur level of both the summer and winter sulfur levels: 161.2 ppm. The average calcium emissions and fuel consumption were calculated using all 99 vehicles selected for chemical analysis in the Kansas City study. The means were calculated using a VMT-weighting, and an equal weight to both the summer and winter data. The VMT weighting places most of the weight on the 1996-2004 vehicles.

To estimate the relative oil and fuel contribution from fleet-average emissions, the model coefficients were adjusted to account for different sulfate formation rates. Both the parameters (β_1, β_2) were adjusted equally with a sulfate conversion adjustment, (α), such that estimated the fleet-weighted sulfate emissions data.

$$\alpha \cdot \beta_1 \cdot \overline{OSE}_{KC} + \alpha \cdot \beta_2 \cdot \overline{FSC}_{KC} = \overline{SES}_{KC} \quad \text{Equation A-3}$$

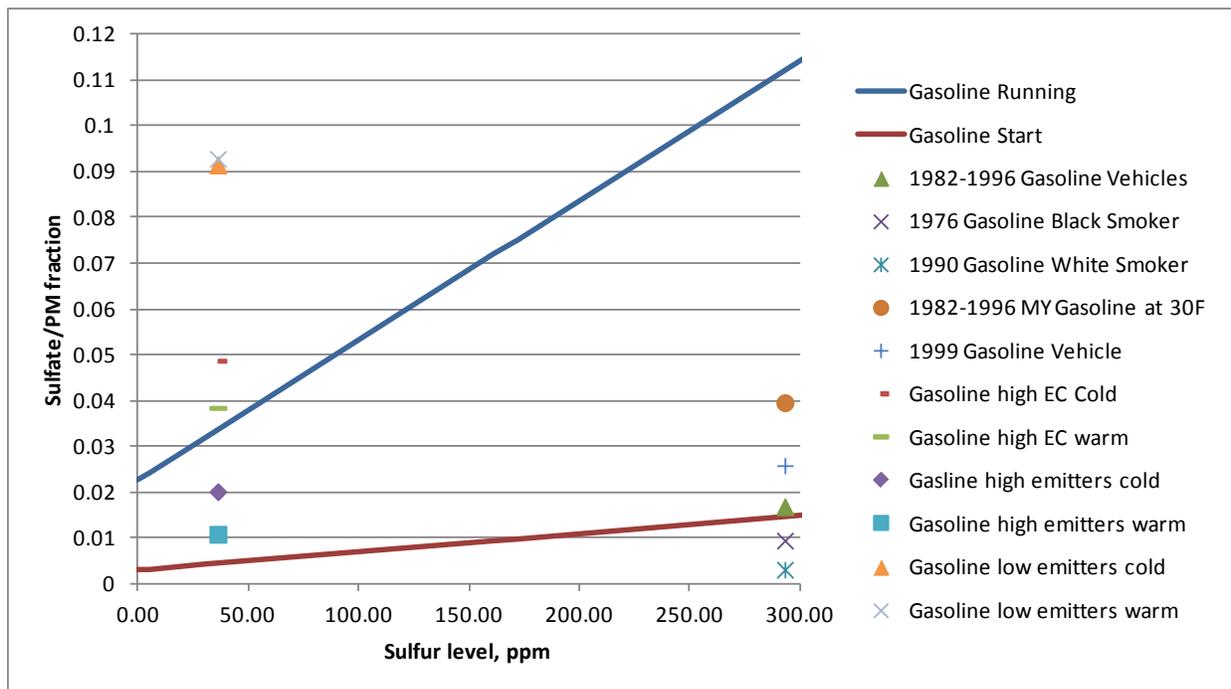
An adjustment value of 1.726 was estimated to fit the VMT-weighted average, meaning that the sulfur in the fuel and oil is 1.7 times as likely to form sulfate emissions using the fleet-average KCVES data set compared to only the summer 1996-2004 vehicles. The increase could be due to increase in oil emissions with older vehicles and the use of oxidation catalysts in older vehicles which increase the formation of sulfate emissions. Table 2-2 displays the estimated fuel sulfate contribution and oil contribution for the VMT-weighted KCVES data. In the KCVES study, 68.7% of the sulfate emissions are estimated to be originating from the gasoline fuel at the observed sulfur level. In MOVES2014, the fuel sulfate contribution (68.7%) scales linearly with changes in fuel sulfur level, but the MOVES2014 retains the lubricating oil sulfate contribution regardless of the fuel sulfur level. The sulfur levels (x_B), and the fuel sulfate contribution values (F_B) in Table A-2 for the fleet results are the parameters that are used in MOVES2014 to adjust the gasoline sulfate emissions (Table 9-1).

A.2.3 Gasoline Model Evaluation

Figure A-2 contains the sulfate models sulfate/PM predictions for gasoline start and running conditions compared to values observed in the literature. The values at 293 ppm sulfur level are obtained from Zielinska et al. (2004⁸⁴). The vehicles were tested in San Antonio, Texas around 1999-2000, with the lubricating oil and commercial fuel “as received.” For comparison with the sulfate values, we assumed that the tested vehicles by Zielinska et al. (2004⁸⁴) had a sulfur value of 293 ppm (obtained from the MOVES2014 default gasoline fuel formulation for San Antonio for calendar years 1999-2000).

The values at 36 ppm sulfur level are obtained from Fujita et al. (2007⁸⁵) from testing of 57 light-duty gasoline vehicles in the DOE Gasoline/Diesel PM Split study, conducted in the summer of 2001. The vehicles were also tested “as received” and gasoline sulfur level was not reported for by Fujita et al. (2007⁸⁵). We estimated the sulfur content for California fuels in 2001, from MOVES default database as 36 ppm.

Figure A-2. Sulfate/PM fractions estimated by MOVES for gasoline vehicles compared to values reported by Zielinska et al. (2004) and Fujita et al. (2007).



We reviewed newer data sources that reported sulfate and PM emission rates from gasoline vehicles. Robert et al. (2007⁸⁶) reported sulfate emission rates from different gasoline technologies ranging from 0.06 ug/km to 3 ug/km fueled on 35 ppm sulfur fuel, which comprised less than 0.0004 as a fraction of the PM_{1.8} emission rates. On the other hand, Cheung et al. (2009⁸⁷) reported sulfate emissions from a Toyota Corolla which had sulfate emissions of 990 ug/km, which composed as a fraction 0.41 of the measured PM emissions. The sulfate values from the FUL were 25 ug/mile, and the fleet-averaged Kansas City Study were 340 ug/mile. Recent testing of sixty-four LDGV vehicles tested at CARB on 1987-2012 model year vehicles indicate that a significant fraction of the PM emissions is composed of ions (<20%) but the sulfate ion fraction of the PM was not reported.⁸⁸

There is a large variation of sulfate emissions reported in the literature (values of sulfate emission rates ranging 4 orders of magnitude). Differences in measurement methods between laboratories on particulate matter and sulfate measurements, and variability in emissions from vehicles appear to contribute to significant variability between the sulfate measurements between the two laboratories. Given the uncertainty, the sulfate model implemented in MOVES2014 still provides results that are within the range of results from the literature.

A.3 Derivation of the Sulfate Calculator Parameters for Conventional Diesel Vehicles

In Phase 1 of the DECSE⁷⁶, two engines were tested with diesel oxidation catalysts: a 1999 Cummins ISM370 and a 1999 Navistar T443 engine. The Cummins is a heavy-duty diesel engine, and the Navistar is a medium-duty engine used in light duty trucks. The engines were tested on steady-state 4-mode test cycles, as well as a transient FTP hot-cycle test. The engines were tested at 4 sulfur fuel levels: 3, 30, 150, and 350 ppm. The lubricating oil used in the study was Shell Rotella T15W40, which is a commercially available CH-4 diesel lubricating oil specified for use in diesel trucks running on sulfur fuel <500 ppm, and engines that comply with the 1998 US EPA engine standards. The sulfur content of the engine oil was measured at 3520 ppm (DECSE phase 1). The PM and sulfate emissions were measured engine-out, and post-catalyst to examine the impact of the diesel oxidation catalyst on emissions. The engine-out and post-catalyst SO₄ emissions are plotted at the four sulfur levels in Figure A-3 and Figure A-4.

Figure A-3. Engine-out sulfate emissions at four fuel sulfur levels (3, 30, 150, 350) measured on a 4-mode and FTP engine test cycle, from a heavy-duty engine (Cummins) and a medium-duty engine (Navistar) from the DECSE Phase 1 Study⁷⁶

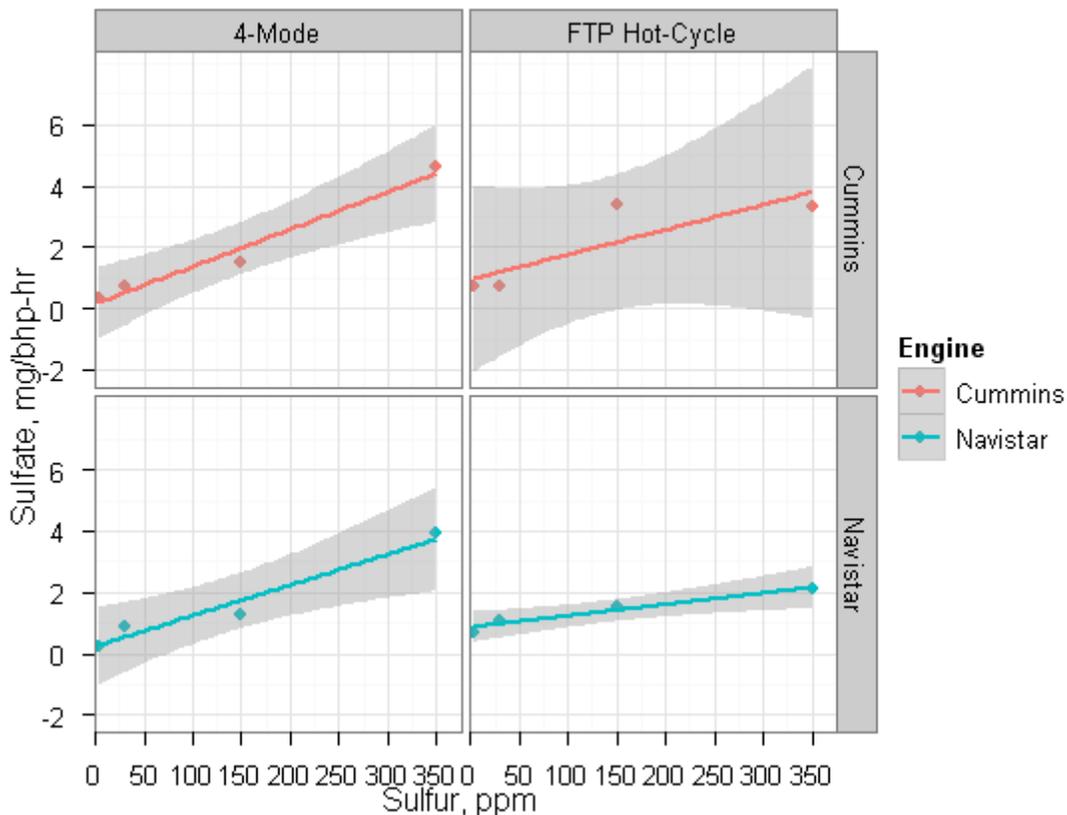
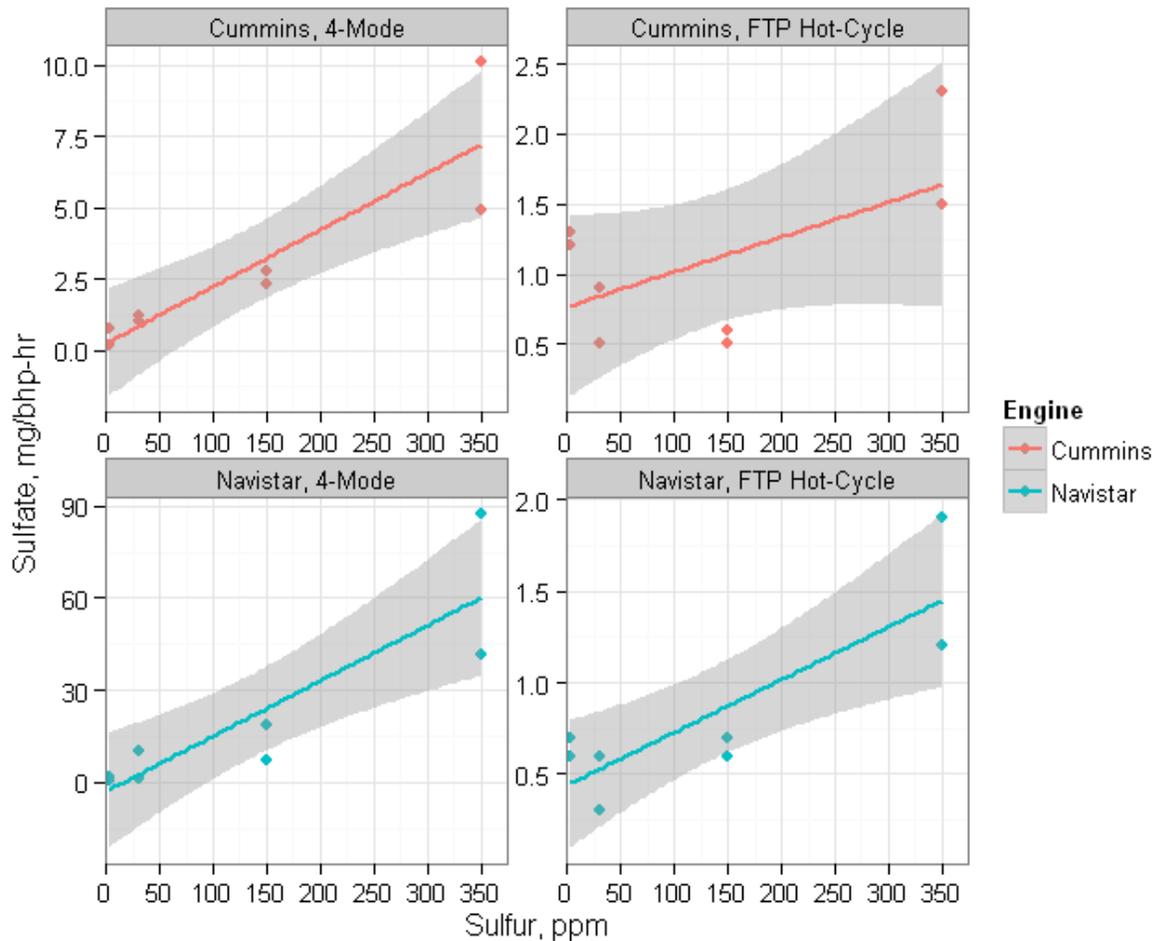


Figure A-4. Post-catalyst sulfate emissions at four fuel sulfur levels (3, 30, 150, 350) measured on a 4-mode and FTP engine test cycle, from a heavy-duty engine (Cummins) and a medium-duty engine (Navistar) from the DESCE Phase 1 Study.⁷⁶



The post-catalyst results produced much more variable results with respect to fuel sulfur. On the steady-state cycle, the medium-duty engine was very sensitive to fuels sulfur level, and produced over 90 mg/mile of Sulfur at the elevated fuel sulfur level. The engine-out results (Figure A-3) produced more consistent results between driving cycles and between the heavy-duty and medium-duty engines. Because this data produced more consistent results, the engine-out sulfate data is used to estimate the relative contribution of lubricating oil and fuel to the sulfate emissions for diesel engines in MOVES. Figure A-5 plots the engine-out sulfate results with respect to fuel sulfur level for the two engines and two driving cycles.

Figure A-5. Simple linear regression fit of the engine-out sulfate emissions and fuel sulfur level data. This includes the medium and heavy-duty engine, and both the steady-state 4-mode cycles and the FTP cycles. The shaded areas are the 95% confidence intervals of the mean-value of the regression.

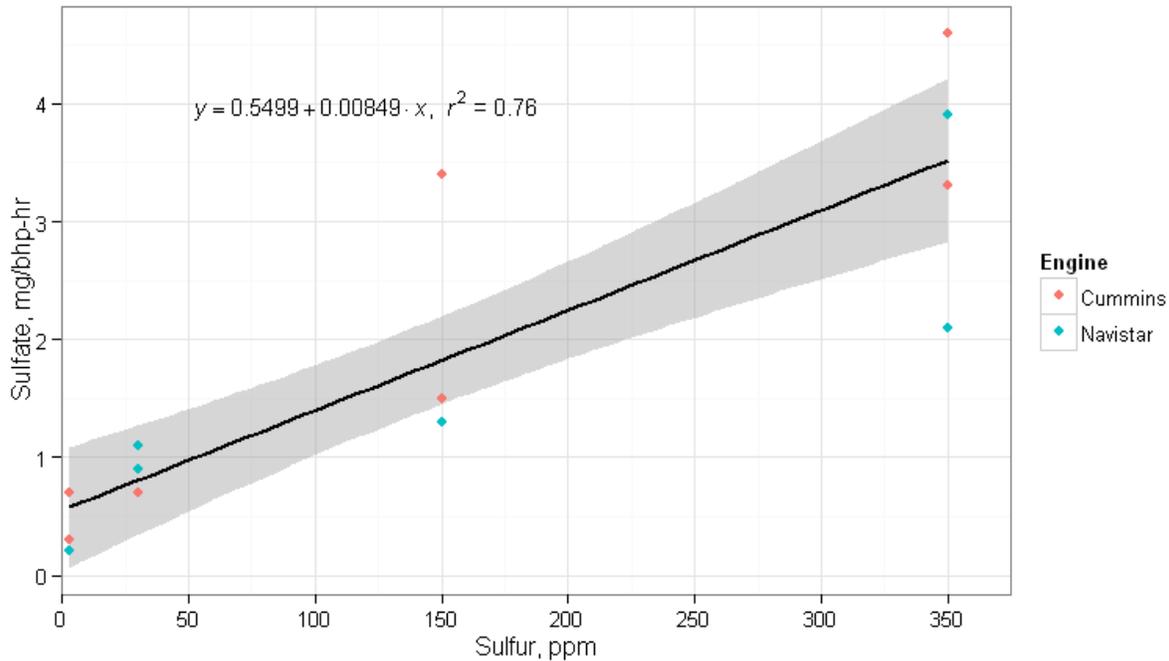


Table 3-1.

Table A-3. Estimated linear regression parameters of the engine-out sulfate emissions and fuel sulfur level data for the data displayed in Figure A-5.

Parameter	Estimate	Std. Error	Lower 95% CI	Upper 95% CI	t-value	p-value
Intercept	0.549904	0.241605	0.0317	1.068	2.276	0.0391
Fuel Sulfur	0.00849	0.001265	0.0058	0.011	6.712	9.92E-06

Using the simple linear regression fit, the relationship between sulfur content and fuel is estimated. The intercept can be interpreted as the sulfate contribution from the lubricating oil.⁶⁹ Using the model coefficients in Figure A-5, the fuel sulfate and oil sulfate contributions are calculated for four sulfur levels in Table A-3 (0, 11, 172, and 350). At 0 ppm sulfur, the fuel sulfate contribution is 0, and all the estimated sulfur is from the lubricating oil. At 350 ppm fuel sulfur, most of the estimated sulfate is from the fuel sulfur. The national default fuel sulfur level in MOVES for heavy-duty trucks is 11 ppm. The estimated sulfur content for the base PM rates for pre-2007 model year diesel vehicles in MOVES is 127 ppm, which is based on the E55/59 study. In MOVES runs, the estimated fuel sulfate contribution from the E55/59 (72.6%) is scaled linearly with changes in fuel sulfur from 172 ppm. We provided the linear model parameter estimates in Table A-3 so that a measure of uncertainty of the derived model coefficients in Table A-4 can be estimated.

Table A-4. Estimated oil and fuel sulfate contributions to the model.

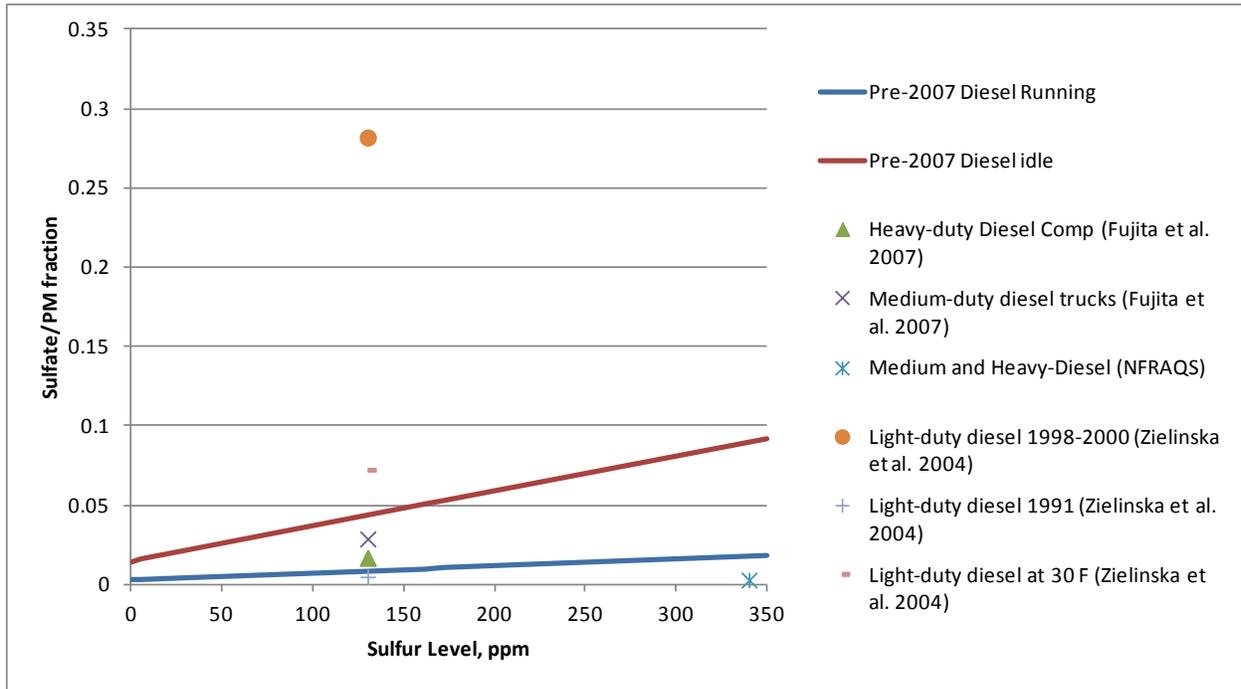
Component	Sulfur level, ppm (x)			
	0	11	172	350
Oil Sulfate Contribution (mg/bhp-hr)	0.55	0.55	0.55	0.55
Fuel Sulfate Contribution (mg/bhp-hr)	0.00	0.09	1.46	2.97
Oil Sulfate Contribution (%)	100.0%	85.5%	27.4%	15.6%
Fuel Sulfate Contribution (%)	0.0%	14.5%	72.6%	84.4%

A.3.1 Pre-2007 Diesel Model Evaluation

In Figure A-6 we compared the estimated sulfate/PM fractions obtained from applying the sulfate calculator in conjunction with the pre-2007 PM speciation profile used in MOVES. We compared these values to values reported for light-duty diesel trucks reported by Zielinska et al. (2004⁸⁴), and from heavy and medium-duty diesel trucks tested as part of the DOE Gasoline/Diesel PM Split Study reported by Fujita et al. (2007⁸⁵). In both of these test programs, the fuel sulfur level was not reported, and the vehicles were tested with the fuel “as received.” For these test programs conducted in 1999-2001 time-frame, the MOVES default sulfur level is 130 ppm for these locations (San Antonio, TX and Riverside CA, respectively). We also compared these values to the sulfate fraction reported in PM_{2.5} SPECIATE profile # 91106 based on the Northern Front Range Air Quality Study (NFRAQS). The diesel fuel sulfur was estimated to be around ~ 340 ppm from three diesel samples taken from three nearby fueling stations.⁸⁹

The sulfate/PM fractions from the literature bound the sulfate calculator predictions in MOVES. Two of the three light-duty diesel sulfate/PM fractions are much higher than the medium-duty and heavy-duty diesel emission rates and from the values predicted from the sulfate calculator and the pre-2007 PM_{2.5} speciation profiles. This may be indicative of a significant differences between light-duty and heavy-duty PM_{2.5} speciation. This could be an area for future research. For now, the sulfate calculator appears to provide a reasonable sulfate/PM fractions compared to the available sources in the literature.

Figure A-6. Sulfate/PM fractions estimated by MOVES for gasoline vehicles compared to values reported by SPECIATE Profile #91106 (NFRAQS), Zielinska et al. (2004⁸⁴), and Fujita et al. (2007⁸⁵).



A.4 Derivation of the Sulfate Calculator Parameters for 2007 and later Diesel Vehicles

Table A-5. Model Parameters for predicting particle number contribution from sulfur in the fuel and the lubricating oil from Kittelson et al. (2008⁶⁷)

Parameter	Estimate	90% Confidence Intervals
Fuel sulfur concentration	36.2	(24.3 to 48.1)
Lubricating Oil concentration	0.142	(0.054 to 0.23)

The relative contributions of sulfate emissions are computed using the contributions from fuel and oil parameters from Table A-5. Table A-6 displays the contributions from lubricating oil, assuming 3,000 ppm sulfur content, and varying levels of sulfur content in the diesel fuel. 4.5 ppm is selected because it is the fuel sulfur level used in the ACES phase 1 program, from which the sulfate emissions for post-2007 emissions are derived. Fifteen ppm is the sulfur limit mandated by the 2007 ultra-low fuel sulfur. The current default sulfur content is 11 ppm used in MOVES2014. As shown in Table A-6, the lubricating oil is estimated to contribute the majority of sulfate emissions when the fuel sulfur level is below 12 ppm.

Table A-6. Estimation of the relative contribution of fuel sulfur and lubricating oil sulfur on sulfate emissions

Parameter	Sulfur level (x) ppm		
	4.5	11	15
Oil Particle Number Contribution (CPC/cm ³)/10 ⁶	426.00	426.00	426.00
Fuel Particle Number Contribution (CPC/cm ³)/10 ⁶	162.90	398.20	543.00
Oil Sulfate Contribution (%)	72.3%	51.7%	44.0%
Fuel Sulfate Contribution (%)	27.7%	48.3%	56.0%

No additional studies were available at the time of this analysis to validate the sulfate model with 2007+ technology diesel engines.

Appendix B Peer Review Comments and Responses

Prior to the release of MOVES2014, this report underwent external peer-review at the end of 2013. We received the compiled comments from the peer-reviewers in early February, 2014.

The two peer-reviewers were:

Tom Durbin, PhD.
Research Engineer
Bournes College of Engineering
Center for Environmental Research and Technology (CE-CERT)
University of California, Riverside

Allen Robinson, PhD.
Raymond J. Lane Distinguished Professor and Head, Department of Mechanical Engineering
Professor, Department of Engineering and Public Policy
Carnegie Mellon University

The peer-reviewers were charged with peer-reviewing chapters from the MOVES2014 Fuel Effects Report that included algorithm and data updates, these document sections included:

- Chapter 3: Fuel Sulfur Effects
- Chapter 6: Gasoline Fuel Effects for Vehicles certified to Tier-2 Standards
- Chapter 9: Sulfate Emissions

An additional chapter (Chapter 7: High-Level Ethanol Blends) describes new data and methods for modeling emissions from flex-fuel vehicles. However, this chapter was not included in the peer-review. The content in this chapter was subject to public review and comment during the Tier 3 Vehicle Emission and Fuel Standards Program.^e

In addition to peer-reviewing updated chapters from Fuel Effects Reports, the peer-reviewers were charged with peer-reviewing two other MOVES2014 Reports:

- Air Toxic Emissions from On-road Vehicles in MOVES2014 Air Toxic Emissions from On-road Vehicles in MOVES2014^f

^e USEPA Office of Transportation and Air Quality. *Updates to MOVES for Tier 3 FRM Analyses*. Memorandum to Docket EPA-HQ-OAR-2011-0135, Item No. 5063. Assessment and Standards Division, Ann Arbor, MI. February 27, 2014.

^f USEPA Office of Transportation and Air Quality. *Air Toxic Emissions from On-road Vehicles in MOVES2014*. EPA-420-R-15-021. Assessment and Standards Division, Ann Arbor, MI. November, 2015.

- Speciation of Total Organic Gas and Particulate Matter Emissions from On-road Vehicles in MOVES2014[§]

The peer-reviewers were also charged to peer-review sections in the following two reports that pertained to speciation updates:

- Exhaust Emission Rates for Light-Duty On-road Vehicles in MOVES2014
- Section 2.3 Estimating Elemental Carbon Fractions
- Section 2.5 Updates to PM_{2.5} emission rates in MOVES2014
- Exhaust Emission Rates for Heavy-Duty On-road Vehicles in MOVES2014
- Section 2.1.2.3.5 Computation of Elemental Carbon and Non-Elemental Carbon Emission Factors

This Appendix provides the list of peer reviewer comments pertaining to the Fuel Effects chapters. Additionally, the peer-reviewers provided ‘general/catch-all’ comments pertaining to all the documents they reviewed. Those general comments are contained in this peer-review, even though they may refer to content in the other MOVES2014 reports. The peer-review comments given specifically with regard to the other MOVES2014 reports are addressed in the appendices of the respective reports.

Reviewers’ Responses to Charge Questions

B.1 All Documents Reviewed

This section provides a verbatim list of peer reviewer comments submitted in response to the general/catch-all review charge question for all documents reviewed as a part of the Fuel Effects, Toxics Emissions, Total Organic Gases (TOG) and Particulate Matter (PM) Speciation Analysis.

B.1.1 Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

[§] USEPA Office of Transportation and Air Quality. *Speciation of Total Organic Gas and Particulate Matter Emissions from On-road Vehicles in MOVES2014*. EPA-420-R-15-022. Assessment and Standards Division, Ann Arbor, MI. November, 2015.

B.1.1.1 Dr. Tom Durbin

This particular question I will address globally for all of the reports, as many of the datasets being recommended apply to more than one report. This is also the area of my significant criticisms. The data sets selected for the MOVES2014 development are large, relatively comprehensive, representative, and generally well conducted, and as such represent a good basis in the model development for MOVES2014. These data sets focus predominantly on the EPA Kansas City study, the E-55/59 study, the ACES Phase 1 study, and the EAct study for fuel effects.

On the other hand, EPA coverage of data is relatively narrow in terms of the larger body of literature, and in particular doesn't consider the relatively significant work being carried out in California. As the MOVES model continues to develop into future years, it is suggested that EPA broadens its coverage of data being collected around the country. Many of the California datasets are just being completed and should be available in time for the next MOVES update.

The issue with the silicone in the Kansas City study for the hot running is another point of consideration. While some corrections can be applied to species profiles that may be reasonable, it also reinforces the idea that a broader range of data sources should be considered.

RESPONSE: We are eager to acquire additional data that would shed light on the behavior of emissions in the model.

Some of the areas where additional data could be particularly useful is for vehicle categories for which data is still relatively limited. In particular, gasoline direct injection engines (GDI) are rapidly expanding into the in-use fleet, have considerably different characteristics compared to more traditional gasoline vehicles, and are not included in the data sets currently being used for MOVES2014. Data for heavy-duty vehicles/engines with newer 2007+ and 2010+ are also still relatively limited. Finally, data on natural gas vehicles/engines are relatively limited.

RESPONSE: Considering the anticipated importance of GDI vehicles in the next decade, research is planned to characterize the effects of fuel properties in vehicles using this technology.

It's difficult to determine how recent the Predictive/Complex model are. In one of the document that discusses fuel effects for sulfur it seems to rely heavily on studies conducted in the early 1990s by CRC and EPA and then goes to the EAct Study with almost no consideration of anything done in between. CARB, on the other hand, considered a number of additional and robust dataset in its 2007 update of its predictive model.

RESPONSE: see response on page 143 below.

Another important consideration is that the heavy-duty pre-2007 data does not seem to include any data from retrofit DPFs, which tend to be more passive in nature and can vary from the OEM DPFs for 2007+ engines.

RESPONSE: The reviewer is correct in that heavy-duty pre-2007 emission rates and accompanying speciation profiles in MOVES are not based on vehicles retrofit with diesel particle filters. MOVES considers pre-2007 vehicles without retrofit technology as the baseline from which users can estimate the benefit of retrofits with knowledge of the retrofit penetration (or expected penetration). The technical guidance regarding modeling retrofits in MOVES is located in the report: Diesel Retrofits: Quantifying and Using Their Emission Benefits in SIPs and Conformity - Guidance for State and Local Air and Transportation Agencies, posted here: <http://www.epa.gov/otaq/stateresources/transconf/policy.htm>. Incorporating a default retrofit penetration in MOVES, along with accompanying emission rate and speciation profiles for pre-2007 vehicles could be considered for a future update.

For the “Gasoline Fuel Effects for Vehicles Certified to Tier-2 Standards” report, there are several other data sets should be considered for inclusion in the fuel effects part of the model as the model continues to be developed. These include the CRC E-83 project, which utilizes the same vehicle fleet as the main EPAAct study, but evaluated fuel olefin levels. UC Riverside is also conducted an extensive study of ethanol/butanol blends that is nearing completion. In particular, this study includes GDI vehicles that are not covered in EPAAct study. This study has some emphasis on California fuels, but should also have more general applicability for evaluated fuels at a national level.

RESPONSE: The studies cited lack sufficient numbers of fuels or an experimental design that would allow them to be directly incorporated into the statistical modeling used to develop the fuel adjustments. Specifically, the CRC E-83 project incorporated only two fuels, with high and low olefins, respectively. It is not possible to simply fold additional datasets into the statistical modeling performed for EPAAct without obviating the experimental design that enables the statistical modeling to be performed in a meaningful way. However, additional studies such as these can be analyzed and evaluated independently for purposes of comparison or verification.

For the “MOVES2014 Sulfate and Sulfur Dioxide Emissions Calculator” report, there are several other data sets should be considered for inclusion in the model as the model continues to be developed. There are several other datasets that are coming out that would be worth EPA considering or at least evaluating with respect to the model, especially on the diesel vehicle side. The California Air Resources Board has been looking at the toxicity of advanced technology vehicles, and some of this data has sulfate emissions that could be of relevance here. The South Coast Air Quality Management District has also conducted a study to evaluate the in-use emission rates of 2007+ technology, heavy-duty diesel and natural gas vehicles. These data will probably not be available until the first part of next year, but they could be considered for future application to the model. Phase 2 of the ACES program is another data set that could be of value for future model revisions.

RESPONSE: As these data will not be available in a timely way prior to model release, it is not feasible to incorporate them into MOVES2014. However, it may be possible to consider them in development of inputs for future releases.

For the “Calculating the Effects of Gasoline Sulfur on Exhaust Emissions” report, there are several other data sets should be considered for inclusion in the model as the model continues to be developed. Even though M6Sulf is supposed to model Tier 1, LEV, and ULEV vehicles, the majority of the datasets listed are from studies conducted in the early 1990s. Given that early 1990s technologies are not very representative of Tier 1, LEV, and ULEV vehicles, consideration should be given to incorporating more data here. Example data sets include the CRC E-60 program.

RESPONSE: In fact, the updated T2Sulf adjustments are applied to gasoline vehicles in model years 2001 and later. Thus, the updated adjustments are applied to LEV and ULEV vehicles, although not to Tier 1 vehicles. Given that it is adapted from the MOBILE model and that it is very dated, and given its complexity, we do not anticipated devoted additional effort or resources to updating the M6Sulf model.

General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

B.1.1.2 Dr. Allen Robinson

Overall I think that EPA has done a good job of developing MOVES2014 and that these chapters provide the reader/user a reasonable description of the model. The models are statistical fits of data; that is probably the best approach given the limitations in our quantitative understanding in the underlying physical and chemical processes that control the emissions. For the most part the models seem to be based on the best available datasets, but there are inevitably gaps. In certain instance there appear to be important data that are not incorporated into the analysis. I have provided many comments on individual chapters. The majority of the comments are focused on improving the usability of the materials. However, there are some important scientific shortcomings (treatment of uncertainty, semivolatile PM, and SOA precursors).

Here are the major comments that apply across most if not all of the sections that I read:

Presentation related:

1. Data sources – the various chapters and report often provide references to the underlying data. However, these references often point to large reports (e.g. the EPAct data analysis), which means that the reader may not be able to figure out what specific data were used. I would encourage EPA to be as specific as possible about what data are used. I have often been frustrated trying to figure out the exact data underlying models like MOVES and MOBILE.

RESPONSE: For studies generating very small datasets, it may be possible to list the entire dataset in a table in the report body or in an appendix. Datasets too large to list on a single page, can often be summarized in an aggregate way in tables or in graphs or charts. However, in the MOVES project, many datasets are too large to present directly even as summaries. In such cases, only subsets or examples can be directly presented without making documents unduly lengthy. However, this point is not unique to MOVES reports, but is equally true of articles in the peer-reviewed literature. In the case of the EAct project, the dataset used to develop the fuel adjustments is publicly available for download at: <http://www3.epa.gov/otaq/models/moves/epact.htm>.

2. Examples – I think quantitative examples really help the reader understand the model. These exist in a few chapters but not in most. I would encourage EPA to include more examples which will help the reader understand what MOVES is doing. Pointing the reader to online tools, such as the fuel effects spreadsheet are also useful.

RESPONSE: For the fuel adjustments based on the EAct models, we have extended the discussion of the example to add text, tables and figures to illustrate and explain the application of the models (absent the sulfur adjustment) and calculation of fuel adjustments for NO_x and THC.

- Tables defining all variables – in some chapter many variables are not defined making it difficult for the reader to understand the model. These tables should also indicate which variables are user inputs and which are derived from existing data. For the user inputs, default values should be clearly defined.

RESPONSE: In a model such as MOVES, discussions in the technical reports describe development of inputs stored in the default database, rather than to inputs provided directly by users through the GUI or through run specifications. However, the variables in the input tables often take hundreds to thousands of values, too numerous to simply list in a report table. Nonetheless, in several chapters of this report, we have attempted to be more thorough in identifying specific input tables involved, listing and defining the fields in the tables, and giving readers some sense of the values or ranges of values taken by the inputs.

3. Example results – For the reader it would be useful to provide some sample output from the model to understand the effects. Ideally this would be graphical presentation.

RESPONSE: We agree with the reviewers comment. Graphical presentation of results of the MOVES model or components of the model has been added to some chapters of this report, including Chapter 3 (sulfur effects) and Chapter 6 (Fuel effects for Tier 2 Vehicles).

Content related:

4. Goodness of fit – Given that the models are statistical fits of data, some description is needed in each chapter on how well the model(s) fit the underlying data is important. These could be some sort of statistical measure and/or scatter plots of model predictions versus underlying data.

RESPONSE: Substantial information concerning goodness of fit has been added to the revised report, particularly for the chapters describing effects of sulfur and other fuel properties on Tier 2 vehicles, i.e., Chapters 3.3 and 6, respectively.

5. Uncertainty – There is no discussion of uncertainty of the model predictions. This is my largest substantive concern with the reports. One measure of the uncertainty is the quality of the statistical fit. A better measure is how well the model performs against data that were not used to derive the fitting parameters. I strongly encourage EPA to quantify the uncertainty in the MOVES2014 predictions. Every prediction should be accompanied by a quantitative uncertainty estimate.

RESPONSE: Given the scale and complexity of MOVES, incorporating such calculations in a MOVES run is intractable at present, as they would require additional inputs and complex calculations employing matrix algebra to existing code. In addition, for the uncertainties to be meaningful in a broad context, it would be necessary to propagate the uncertainties in fuel adjustments with the numerous other uncertainties in the calculations. Unfortunately, while the availability of such uncertainty estimates would be valuable, the additional computational burdens involved in multiple propagations of uncertainty would in all likelihood make the use of MOVES infeasible for most users.

6. Data limitations – EPA has done a good job utilizing existing data. However, there are inevitably gaps. Obvious gaps are GDI, higher mileage vehicles, high emitters, etc. The reader should be made aware of these limitations and guidance should be given about how to address.

RESPONSE: The reviewer raises important questions. See discussion on page 144 ff.

B.2 Gasoline Fuel Effects for Vehicles Certified to Tier-2 Standards

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the chapter Gasoline Fuel Effects for Vehicles Certified to Tier-2 Standards, IN: *Modeling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*.

B.2.1 Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

B.2.1.1 Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section B.1.

B.2.1.2 Dr. Allen Robinson

I think that the presentation of the data sources (specifically test fleet, and fuel composition) could be improved. There is a lot of detailed information in the main EPAAct report, which I download and skimmed parts of, but it would helpful for the reader if a bit more information (a few more paragraphs) was provided in the intro about this test program. Here are some examples of the sort of information that would be useful to provide the reader: Were these all relatively new, low-mileage vehicles? What was the variety of emission control technologies? Were the vehicles all port fuel injected? Were all the vehicles 2008 MY? How were the vehicles procured? Recruited from the in-use fleet – if so where? What was the range of each property of the fuels tested in EPAAct? What are typical values for each of these properties in actual in-use fuels (summer and winter)?

If all the vehicles were port fuel injected then what is the guidance for gasoline direct injection vehicles which are becoming more prevalent? That seems like the most significant gap in the information.

All of the EPAAct vehicles were low mileage, what are the recommendations for higher mileage tier 2 vehicles?

These things seem like important data limitations. Although these issues probably cannot be addressed (these types of vehicles were not in the EPAAct test fleet), the document should clearly describe potential limitations of the model so that the reader is aware of them.

RESPONSE: The reviewer's comment is well taken. To address these points we have condensed additional information from the project report and added it to the MOVES report. Among other topics, we have added descriptions of the vehicle sample, test fuels and the study design.

B.2.2 Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

B.2.2.1 Dr. Tom Durbin

The description of the methods and procedures is reasonable. The following are some suggestions in this area.

Section 2.1 should have a reference to a more basic description of the “Z factor” and other elements of the discussion for those looking for a more fundamental discussion of the method.

RESPONSE: Standardization is one of the most common techniques in statistical analysis, serving, for example, as the basis for the Z test between means and t tests of significance for regression coefficients. Nonetheless, we have cited several sources that give descriptions of standardization and some of its applications to allow interested readers to better understand the background of the approaches used in the EPAct analysis.

The first example on page 6 is for aromatics, and then the examples switch to ethanol.

RESPONSE: Yes. The examples are provided not to exhaust all possibilities but rather to illustrate the process more concretely.

Tables 2 and 3 provide a good description of the different coefficients. It is worth noting that because Table 3 is in log scale it, it is not necessarily straightforward to determine the magnitude of the effects that might be seen for different in arithmetic space. It would be interesting to see what the coefficients would be when they are transformed to arithmetic space, although this is not how they are used in the model. Also, the blanks in table 3 are not explained. Tables 5 and 6 are good, especially Table 6 that goes into detail on each of the terms.

RESPONSE: Since the response variable is always the natural logarithm of emissions, it would not be meaningful to attempt to represent the model coefficients themselves in “arithmetic space.” However, model results can be expressed in arithmetic space by applying the reverse exponential transformation. Note that the logarithmic form is convenient in that the arithmetic difference in model results for two fuels represents a ratio difference. The blanks in Table 3 represent terms that were not retained in specific models following model fitting. In the revision we have added a description of the model fitting process and replaced Table 3 with a set of tables that shows the full and reduced models for each combination of pollutant and process (i.e., start, running).

For the means in Table 2, are these based on just a mean for the fuels in the test matrix, or are they weighted based on the number of tests run on each fuel for the dataset being used.

RESPONSE: The means in Table 2 represent the fuel matrix itself and do not incorporate weighting by numbers of replicates on combinations of vehicle and fuel. This approach simplifies both the fitting and application of the models by allowing the same standardization to be used in all cases.

The first example on page 6 is for aromatics, and then the example switches to the quadratic term for ethanol.

RESPONSE: Yes. The examples are provided not to exhaust all possibilities but rather to illustrate the process more concretely.

How are start and running emissions calculated? Based on bag 1 for start and bag 2 for running?

RESPONSE: Correct. "Start" emissions represent Bag 1 of the LA92, and "running" emissions represent Bag 2. Not also that "start" and "cold start" are treated as synonymous, as are the terms "running" and "hot-running." We have added text to the revised chapter to make these points more explicit.

B.2.2.2 Dr. Allen Robinson

The core statistical model/parameterizations appears to have been derived by the EPAct project and appears to be described in the final report for that project (Assessing the Effect of Five Gasoline Properties on Exhaust Emissions from Light-Duty Vehicles Certified to Tier 2 Standards: Analysis of Data from EPAct Phase 3 (EPAct/V2/E-89) Final Report (EPA-420-R-13-002)). In that (EPAct) report they describe multiple models, but the set of parameters that will be used in MOVES2014 appear to be the same as what is listed in Table ES-1 and ES-2 of the EPAct report (the only exception appears to be the value of the variance listed in Table 3 – why are those different?). This was not clear from reading the fuel effects document. If that is the case (the models were taken directly from the EPAct report), then this document needs to have a short declarative sentencing stating so. “The models used here were derived and described in the EPAct final report (ref).” Right now the introduction only provides a very qualitative discussion of the EPAct process, but does not explicitly say that the analysis was used here. If the model is different than one of the models derived in the EPAct report then this report needs a lot more discussion of the derivation of the model.

RESPONSE: It is correct that the models used are those listed in the Executive Summary of the Project Report. We have added text to make this point explicit.

Without reading the EPAct report the reader has essentially no “understanding of the steps taken and assumptions made by EPA to develop the model inputs.” The EPAct report is very long and detailed. In addition, they fit multiple models to the data. This chapter would benefit if it provided some more discussion of the EPAct modeling process and why this particular model was chosen (as opposed to one of the other models fit by the EPAct team). This would be a page or so of text. This would give every reader a basic understanding of the model; interested readers could then be referred to the EPAct report for more details. I thought that the air toxics report did a much better job of describing the underlying model(s) than this chapter.

RESPONSE: The reviewer makes a good observation. To address this deficiency we have added material to give a relatively brief description of the iterative model-fitting processes employed in the project. We believe that the revised text will give general

readers a much better idea of how the models were developed. However, readers desiring in-depth understanding of how the EPAAct analyses were conducted will still need to consult the project reports.

Another shortcoming of this document is that it does not provide some description of the goodness of fit of the model to the original data (part of this should be providing some physical description of what the variance values in Table 3). I skimmed through multiple sections of the EPAAct report and could not find that succinctly summarized. A few paragraph (up to a page or two) description of the goodness of fit of the model to EPAAct data should be provided as the ability of MOVES2014 to predict fuel effects ultimately depends on the model and how well it describes the data.

RESPONSE: In addition to describing the model-fitting process, we have added tables summarizing model coefficients, standard errors and associated t-tests (or χ^2 tests) for individual coefficients. Reviewing these statistics gives a clear sense of how model terms not contributing to fit are dropped during model fitting. Unfortunately, commonly used and easily interpreted goodness-of-fit measures, such as R^2 , are of little use in this context, as the vast majority of variability in the dataset is attributable to differences among the test vehicles. However, the goal of the analysis was to account for the much smaller fraction of variability attributable to differences in fuel properties.

Were any exercises performed to test the model with independent data (data not used to fit the model)? Standard techniques such as “leave-one-out” can be used. Alternatively one could use speciated data from other test campaigns to test the model? For example, ARB has extensive data from their surveillance program. This sort of independent evaluation of the model with real world data seems extremely important. This analysis should be performed and described in the report to provide the user confidence in the model.

RESPONSE: Two projects sponsored by the Coordinating Research Council are playing this role. The first is E-98 (Exhaust Emissions of Average Fuel Composition), in which additional measurements were performed on the sample of vehicles used in EPAAct/V2/E-89, using fuels representing properties in the “envelope of properties defined by the EPAAct fuels.” In addition, the results of E-98 have been applied in E-101, a project designed as a comprehensive evaluation of the MOVES2014 model. A final report for E-101 is expected during 2016.

What was the basis for the assumption “that effects for fuels and temperature are independent and multiplicative.”

RESPONSE: The commenter notes correctly that the datasets used to estimate fuel effects did not incorporate the effect of temperature.

At the outset, we can point out that MOVES does not apply temperature adjustments to hot-running CO, THC or NO_x emissions, thus obviating the need to consider interactions between temperature and fuel effects. That the effect of temperature on hot-running gaseous emissions is negligible is widely accepted.

For start emissions of CO, THC and NO_x, however, MOVES applies both temperature and fuel effects, under an assumption that they can be applied multiplicatively and independently. However, when multiplicative effects are jointly applied to mass emissions (in “linear” as opposed to logarithmic space), the results appear “interactive” in that the different effects either reinforce or damp each other. For example, start emissions increase substantially as temperature declines, with the implication that fuel effects are amplified at lower temperature, whether positive or negative. The net result can be either increased or decreased emissions, depending on the nature of the fuel effects.

We can focus on start CO as an example. For CO (HC and NO_x) fuel effects are calculated using the Complex model for 2000 and earlier model years, and using the EPAAct models for 2001 and later model years. In both cases, the results applied are broadly consistent with those of a past study (CRC E-74b). As the two studies applied differing approaches to statistical analysis, the respective model coefficients cannot be compared in terms of magnitude. However, they can presumably be compared qualitatively in terms of sign.

For cold-start CO emissions (Bag 1), the Complex Model has a small but positive linear-effect coefficient for RVP. This result is directionally similar to the E-74b Composite CO model, which also has positive RVP coefficients, as well as a positive interaction between RVP and temperature. This result implies that for “cold” temperatures below 50°F, increasing RVP should increase CO, with the effect amplified by decreasing temperature. The application of the Complex Model in MOVES gives qualitatively similar results with a positive RVP coefficient amplified by the multiplicative temperature adjustment.

For MY2001 and later, the EPAAct models can be applied to start emissions specifically. The CO start model has a negative linear coefficient for RVP, (meaning that emissions decline as RVP increases). In E-74b, a piece-wise fit was used, giving negative and positive coefficients for RVP < 9 and > 9 psi, respectively. In addition, a positive interaction term was included in the reduced model. As expected, the temperature coefficient is negative, suggesting that an “interference” interaction obtains, i.e., that the combined effects of RVP and temperature would have a mutual “damping” effect. The net results of the E-74b model are shown in Figure 5-1 (page 76). At temperatures below 50 °F, the trends portrayed show an “interference” effect, i.e., that increasing RVP decreases CO start emissions, with the absolute margin (in g/mi) increasing with declining temperature. As mentioned, despite the differences in underlying data and modeling approaches, the application of independent RVP and temperature effects in MOVES gives similar results. This outcome results from the multiplicative combination of a negative temperature effect (CO increases and T decreases) with a negative RVP effect (CO decreases as RVP increases). The net result is that the temperature effect is reduced by increasing RVP at lower temperatures, which is directionally similar to the result obtained in E-74b, and suggested by the commenter as a correct representation of CO behavior in relation to RVP and “cold” temperature.

Results for THC and NO_x are similar. The models applied in MOVES do not contain temperature effects, but multiplicative combinations of the fuel and temperature effects results in interaction effects in the projected emission volumes. Thus, on the whole, we conclude that the multiplicative combination of temperature and fuel effects as applied in MOVES does allow for interactions between these effects.

B.2.3 Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

B.2.3.1 Dr. Tom Durbin

The equations for this report appear to trace back to methods used and reviewed previously. The current application of these methods appears to be appropriate in that context. Comments to consider on the presentation of the methods are provided above.

RESPONSE: In the revision, we have incorporated material from the EAct project report to briefly summarize the EAct project and analyses, including an overview of the test vehicles, test fuels and the model fitting process.

It's difficult to determine how recent the Predictive/Complex model are. In another document that discusses fuel effects for sulfur it seems to rely heavily on studies conducted in the early 1990s by CRC and EPA and then goes to the EAct Study with almost no consideration of anything done in between. CARB, on the other hand, considered a number of additional and robust dataset in its 2007 update of its predictive model.

RESPONSE: The Complex model has not been updated since it was originally developed in the early 1990's. The "EPA Predictive Model," however, was updated in 2001 in the context of EPA's review of California's Request for Waiver of the Reformulated Gasoline Requirement. At that time, additional data was incorporated in the EPA analysis. However, it is not clear that combining other datasets with the EAct dataset would improve the analysis. Incorporating additional data would obviate one of the main advantages of the EAct project, namely, the carefully optimized randomized-block design, which allows substantial vehicle variability to be neutralized in the analysis of fuel effects. In our view, it could be a better use of other datasets to analyze them independently with respect to their own designs and data structures, and to make comparisons to the EAct results.

B.2.3.2 Dr. Allen Robinson

This sort of statistical fitting is commonly done to create "models" to describe fuel effects. The parameters included in the model are known to influence emissions. However, I am not aware of any scientific basis for the underlying mathematical form of the model. If there is one the report would benefit from a description of it. In addition, without the information on goodness of fit

and evaluation of model with independent data as described in the previous section it is impossible to answer these questions.

RESPONSE: The models developed in the project are statistical models in the commonly used sense of the term, and as such, describe associations between fuel properties and emissions. The mathematical forms of the models do not attempt to represent physical processes or relationships. To our knowledge, such forms have never been proposed for the multi-dimensional relationships that were the subjects of study in the EPAAct project. It is important to add that assignment of cause and effect cannot be inferred from the associations themselves and must be supplied through interpretation. (Note that such models are called “linear” because they are linear in their coefficients, not because they necessarily describe straight-line trends). The linear forms of the models are very commonly used in empirical studies and provide a framework within which to analyze and express degrees of association.

Beyond a description of the goodness of fit, the major shortcoming of the model is there is no treatment of uncertainty. I would advocate that the model should provide uncertainty estimates (confidence intervals) for every output/prediction. One simple way to provide an estimate would be to use the statistical uncertainty of the fit. This is reasonably straightforward. A more robust approach would also be to try to account for the limitations in the underlying dataset (e.g. lack of GDI). Providing a robust treatment of uncertainty is not easy but it seems essential to ensure that the data are used appropriately. Including uncertainty estimates would be a major upgrade of the model, which may not be possible for this release of MOVES. However, I would strongly encourage EPA to make starting implementing uncertainty a high priority for future releases.

RESPONSE: Calculations of uncertainty for model predictions can be readily performed, by combining sets of covariances for the model coefficients with sets of properties for the fuel(s) under consideration. Incorporating such calculations in a MOVES run is intractable at present, as they would require additional inputs and complex modifications employing matrix algebra to existing code. In addition, for the uncertainties to be meaningful in a broad context, it would be necessary to propagate the uncertainties in the fuel adjustments with the numerous other uncertainties in the calculations. Unfortunately, while the availability of such uncertainty estimates would be valuable, the additional computational burdens involved in multiple propagations of uncertainty would in all likelihood make the use of MOVES infeasible for most users.

B.2.4 Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

B.2.4.1 Dr. Tom Durbin

This report does not deal extensively on data sets where data is meager. On the other hand, the data set being used does not contain any GDI vehicles, which will represent a growing and important segment of the in-use fleet going into the future.

B.2.4.2 Dr. Allen Robinson

I don't think that there are any statements about data limitations in this section. However, there are some critical data gaps, such as for GDI, higher mileage vehicles, and malfunctioning (gross emitting) Tier2 emitting vehicles. It would be good to at least specifically mention these gaps.

RESPONSE: The importance of these assumptions justifies spending some effort to examine them, and to review available data that has the potential to falsify them.

It is correct that the EPAAct models were developed using a set of low-mileage Tier-2 vehicles, and that in MOVES the models are applied to Tier-2 vehicles as they age and acquire mileage. Nonetheless, we argue that these extrapolations are reasonable and appropriate given the ways in which the models were developed and the fuel adjustments applied.

The comment itself is premised on an assumption that fuel effects should differ in some way between vehicles of differing technologies, ages or "high-emitter" status. Fuel effects are represented in MOVES as multiplicative effects that are proportional to base emission levels. We agree with the reviewer in that when fuel effects are expressed as absolute changes in mass (e.g., g, g/mi, g/kg, etc.), vehicles of different technologies or ages will differ strongly. We do, however, assume that proportional, or relative fuel effects (expressed as fractions, ratios or logarithmic differences), can be seen as similar and thus transportable on average across technology groups and ages.

The data available to directly evaluate this assumption are limited. Nonetheless, some relevant data can be compiled from the results of the EPAAct program. The models applied in MOVES were developed from the results of EPAAct Phase 3, in which 15 Tier-2 vehicles were measured on 27 fuels. In addition, in EPAAct Phase 5, three vehicles manufactured in the 1990's were measured on three fuels used in Phase 3. Thus, using these results, it is possible to make a direct comparison of emissions for sets of pre-T2 and Tier-2 vehicles measured on the same fuels (at 75°F).

The three 1990's vehicles are briefly described in Table R-1. Note that these vehicles range from 10-17 years in age and that all had presumably accumulated over 150,000 mi.

In terms of fuels, we limited the comparison to 2 fuels with 0 and 10% ethanol content, respectively. These two fuels are closely matched in terms of RVP and aromatics levels, and differ slightly in T50. However, they differ widely in T90. The properties of these fuels are summarized in Table R-2. Note that emissions on both fuels were acquired for only two of the three vehicles.

Table R-1. Characteristics of three "High-mileage" pre-Tier-2 Vehicles measured in EPAAct (Phase 5).

Make/Model	Engine	Model Year	Odometer (mi)
Chevrolet Tahoe	V8 – 5.7 L	1997	221,000

Ford Taurus	V6 – 3.0 L	1990	>90,400(?)
Dodge Dakota		1993	229,000

Table R-2. Selected Properties of Two Fuels measured in EPAAct (Phase 5).

Fuel No.	Ethanol (vol.%)	Aromatics (vol. %)	RVP (psi)	T50 (°F)	T90 (°F)
6	10.56	15.0	7.24	188.5	340.4
7	<0.10	17.0	7.15	193.1	298.4

At the outset, we averaged the results by vehicle and fuel, and plotted the results for both cold-start and hot-running phases of the LA92 cycle. Results for NO_x, THC and PM are shown below in Figures R-1 to R-6. Note that the results are shown on a logarithmic scale (base 10). This view of the data facilitates showing the results for all the vehicles in one plot. In addition, differences in logarithms can be interpreted as proportional or relative differences between the fuels for the various vehicles.

Aside from the fact that their emissions are higher, the differences in logarithms between the two fuels are not obvious for the older “high-mileage” vehicles. Although the sample of older vehicles is small, a qualitative view of the plots suggests that no clear and obvious differences between T0, T1 and T2 vehicles are evident.

Figure R-1. NO_x (Bag 1): Mean Emissions for Low mileage Tier-2 Vehicles and high mileage T0 and T1 vehicles on two Fuels.

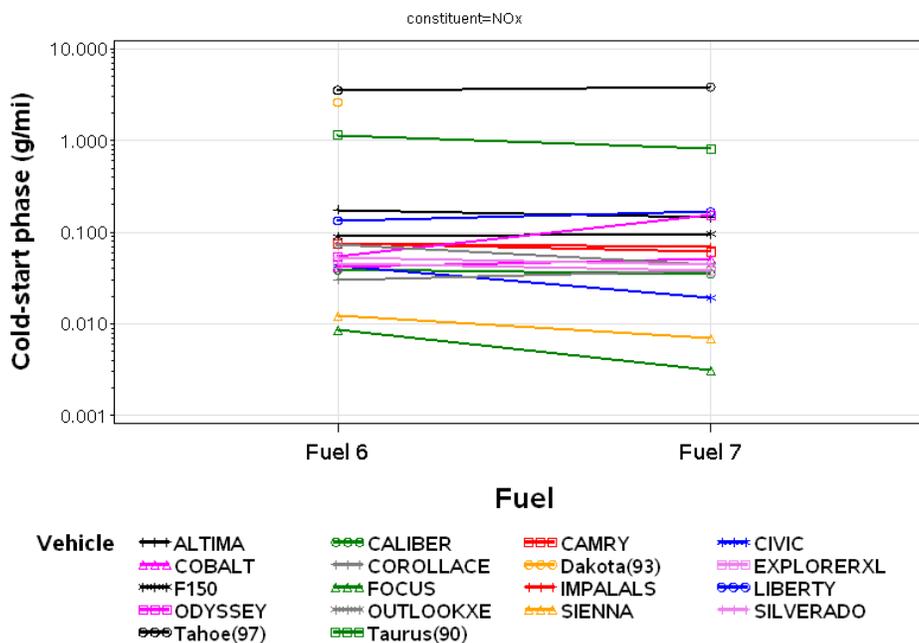


Figure R-2. NOx (Bag 2): Mean Emissions for Low mileage Tier-2 Vehicles and high mileage T0 and T1 vehicles on two Fuels.

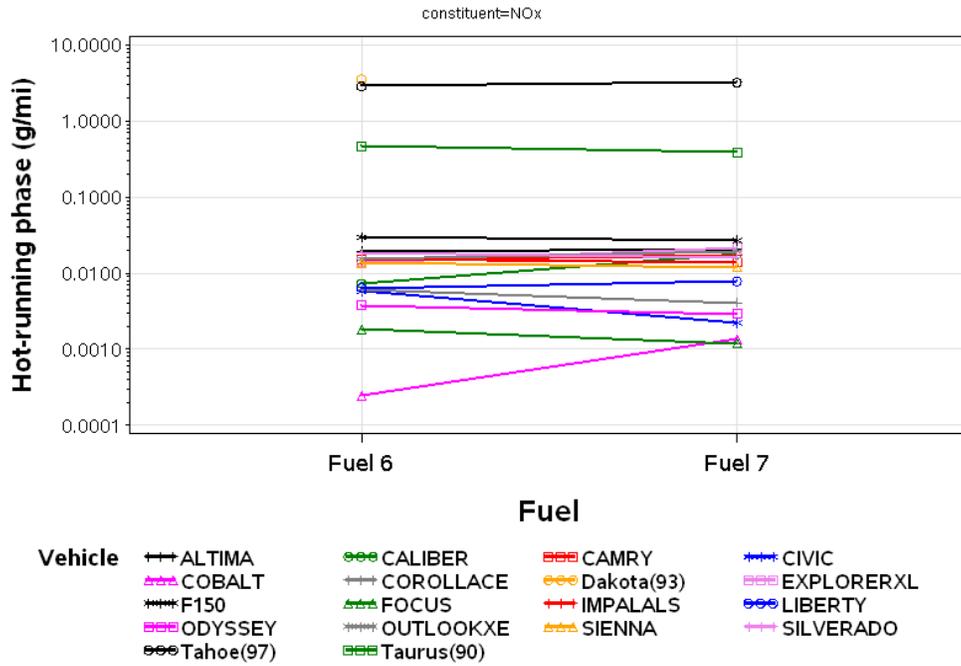


Figure R-3. THC (Bag 1): Mean Emissions for Low mileage Tier-2 Vehicles and high mileage T0 and T1 vehicles on two Fuels.

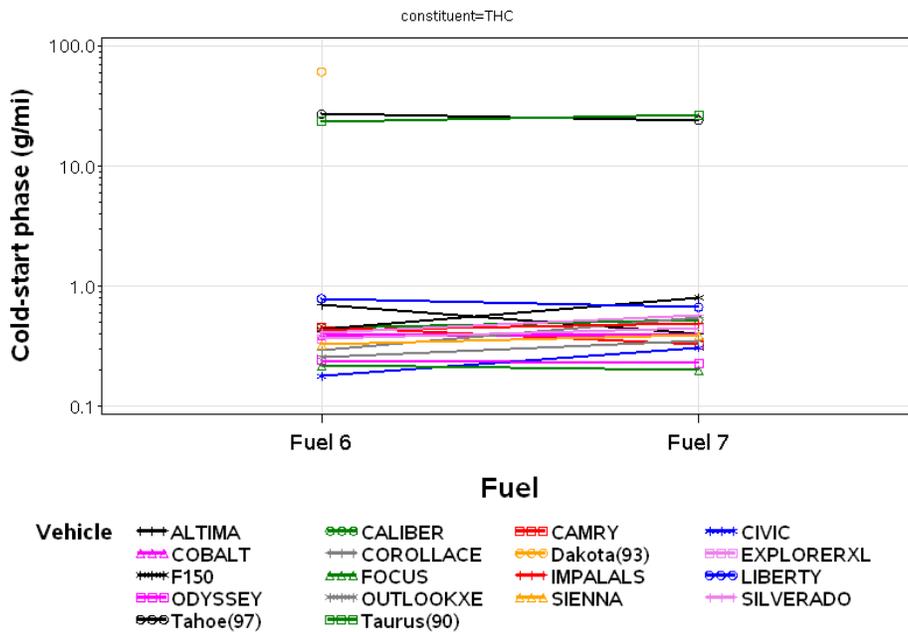


Figure R-4. THC (Bag 2): Mean Emissions for Low mileage Tier-2 Vehicles and high mileage T0 and T1 vehicles on two Fuels.

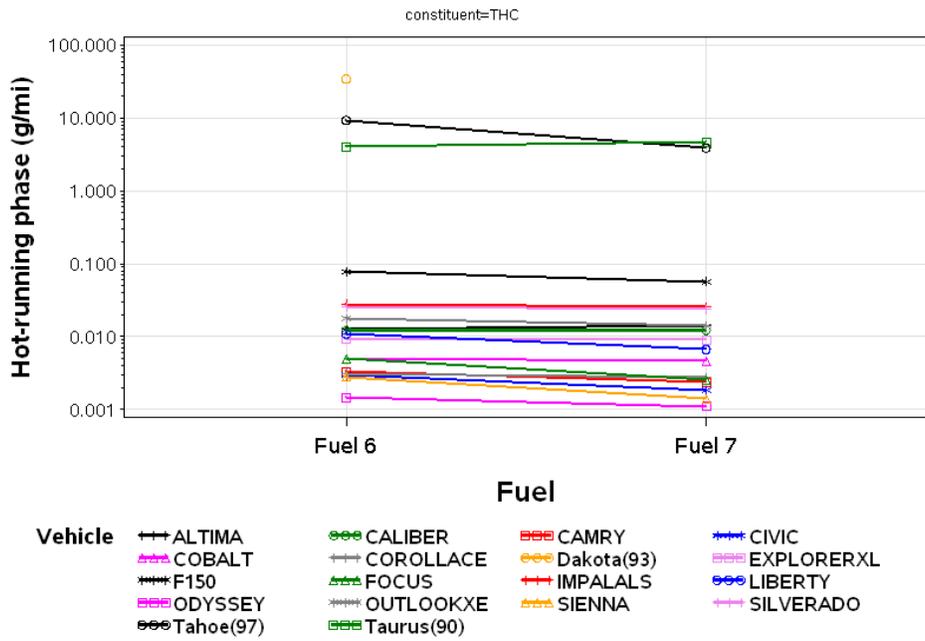


Figure R-5. PM (Bag 1): Mean Emissions for Low mileage Tier-2 Vehicles and high mileage T0 and T1 vehicles on two Fuels.

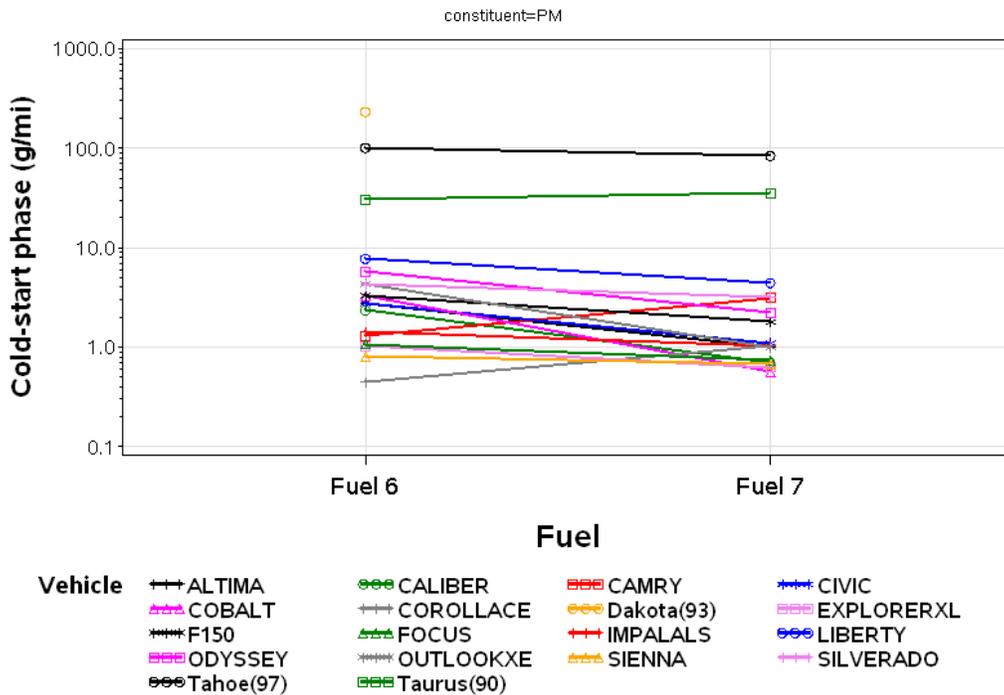
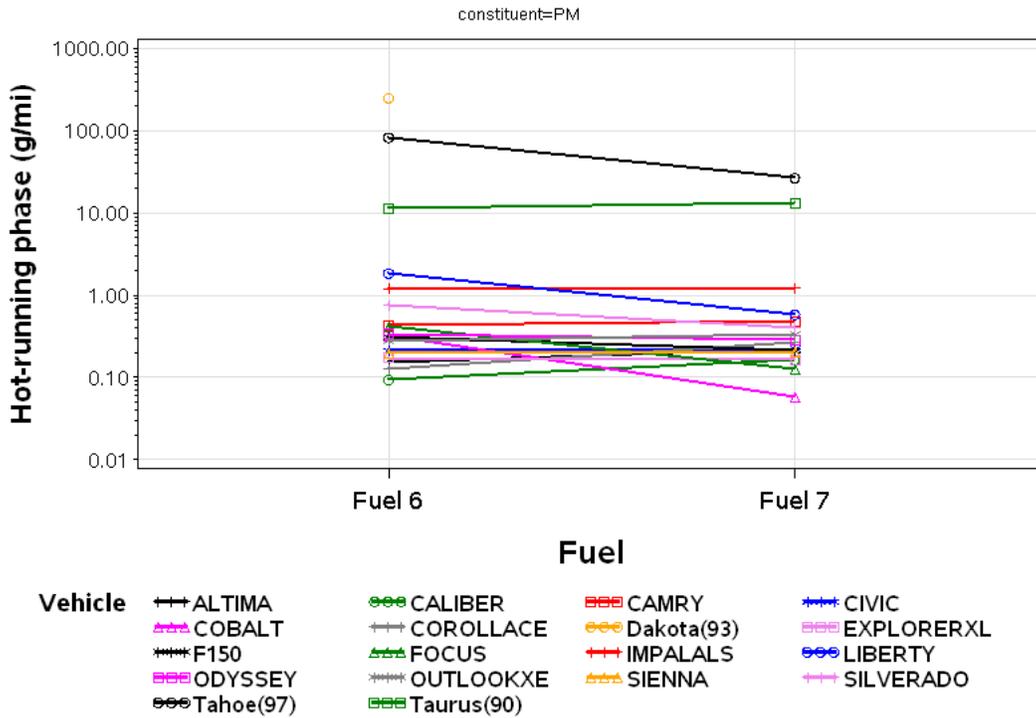


Figure R-6. PM (Bag 2): Mean Emissions for Low mileage Tier-2 Vehicles and high mileage T0 and T1 vehicles on two Fuels.



It is helpful to follow up with a closer examination of this subset of results. As mentioned, differences in logarithms represent ratios, e.g., $\log a - \log b = \log(a/b)$. However, for purposes of summary, it is more intuitive to express the results as percent differences between fuels 6 and 7 (relative to fuel 7). Accordingly, mean percent differences for the set of vehicles are presented below in Figure R-7 to R-9 for NO_x, THC and PM, respectively. In each plot, the differences are ranked from smallest to largest, meaning that the ordering of the vehicles differs in each chart.

In reviewing the charts, it is clear that when the differences in emissions between the two fuels are viewed as fractions, there are no clear or obvious differences between the 1990's vintage high-mileage vehicles and the MY 2008 Tier-2 compliant low-mileage vehicles. Generally, the two high-mileage vehicles differ in the signs of their effects, with one vehicle showing a positive and the other a negative change. Cold-start PM is the only case in which both vehicles have negative effects and have low rankings. Hot-running THC also stands out as the only in which the two older vehicles have the largest and smallest fractional effects. In the remaining cases the older vehicles are distributed evenly across the rank order.

Overall, the available evidence suggests that when fuel effects are expressed as relative multiplicative factors, as they are in both the EPA_{act} analyses, and in their applications in MOVES, it is reasonable to assume that the proportional effects are transportable across different vehicle technologies, as well as across other factors such as age, mileage or "high-emitter" status.

Figure R-7. Mean Percent Difference in NOx Cold-Start (top) and Hot-running (bottom) Emissions from 14 Tier-2 and 2 pre-T2 vehicles measured on two Fuels.

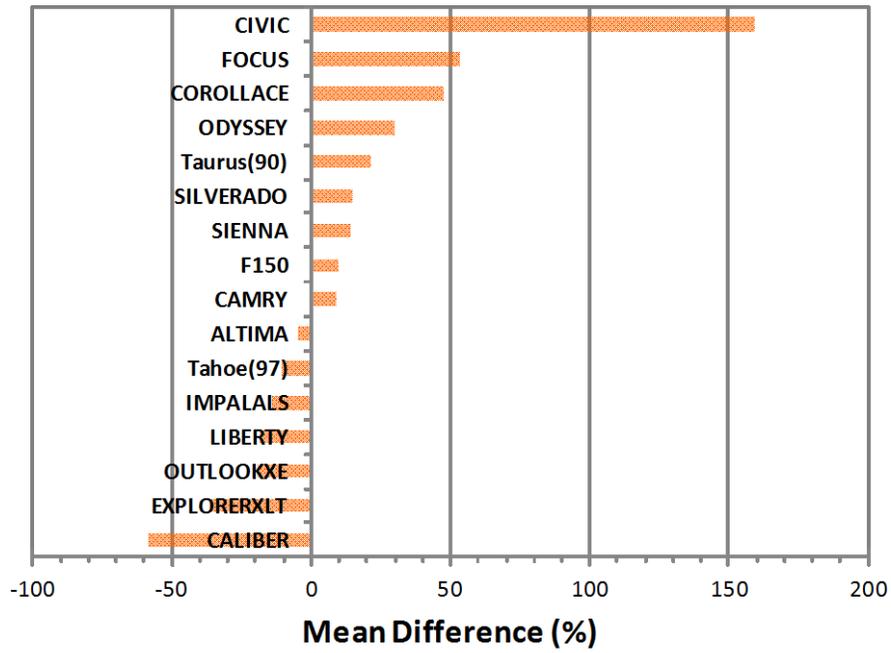
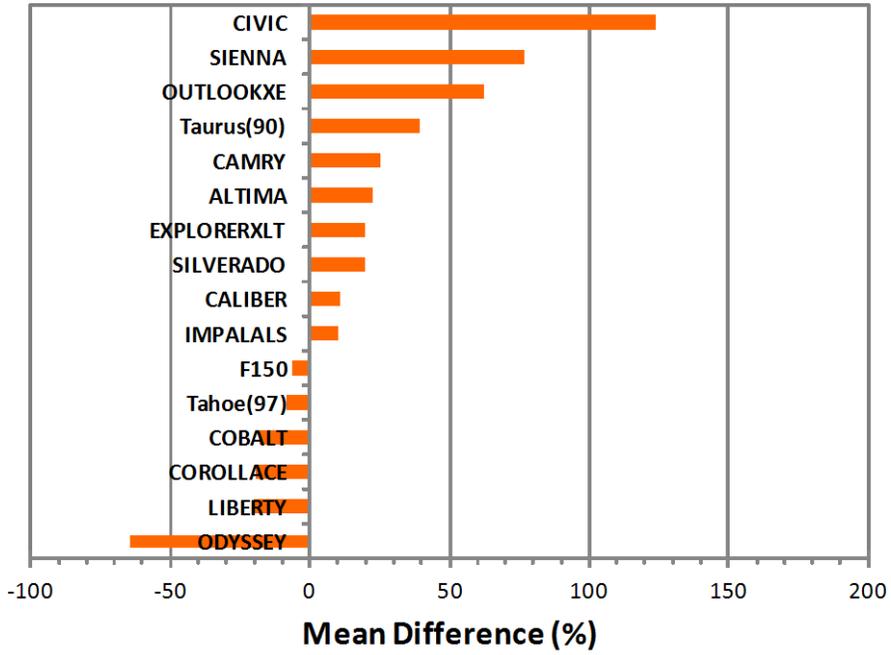


Figure R-8. Mean Percent Difference in THC Cold-Start (top) and Hot-running (bottom) Emissions from 14 Tier-2 and 2 pre-T2 vehicles measured on two Fuels.

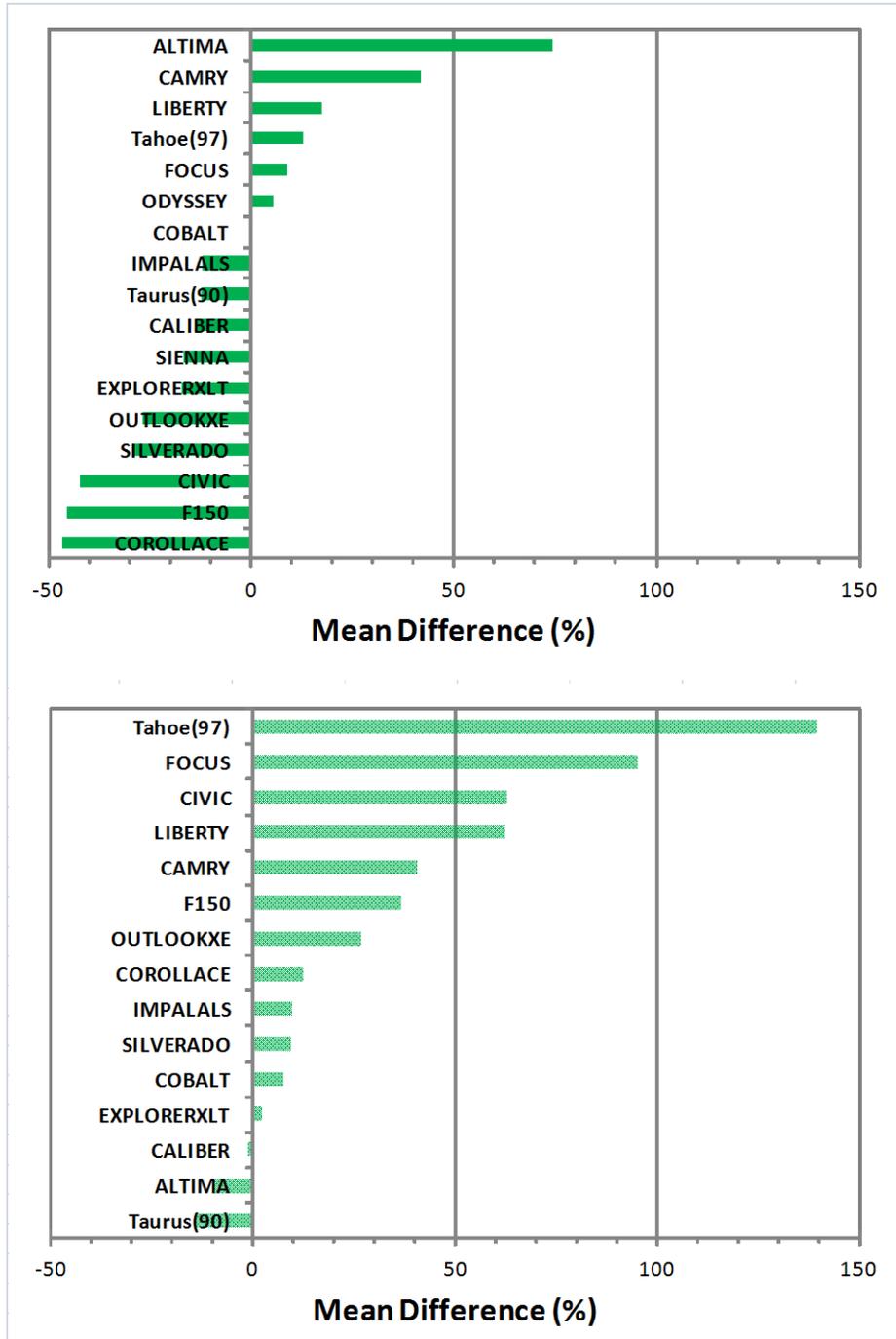
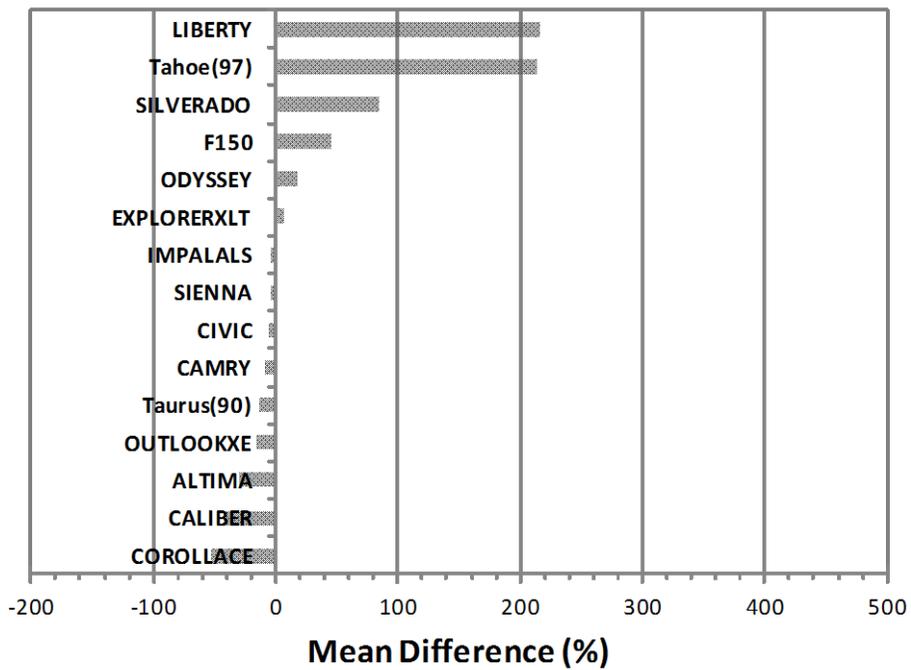
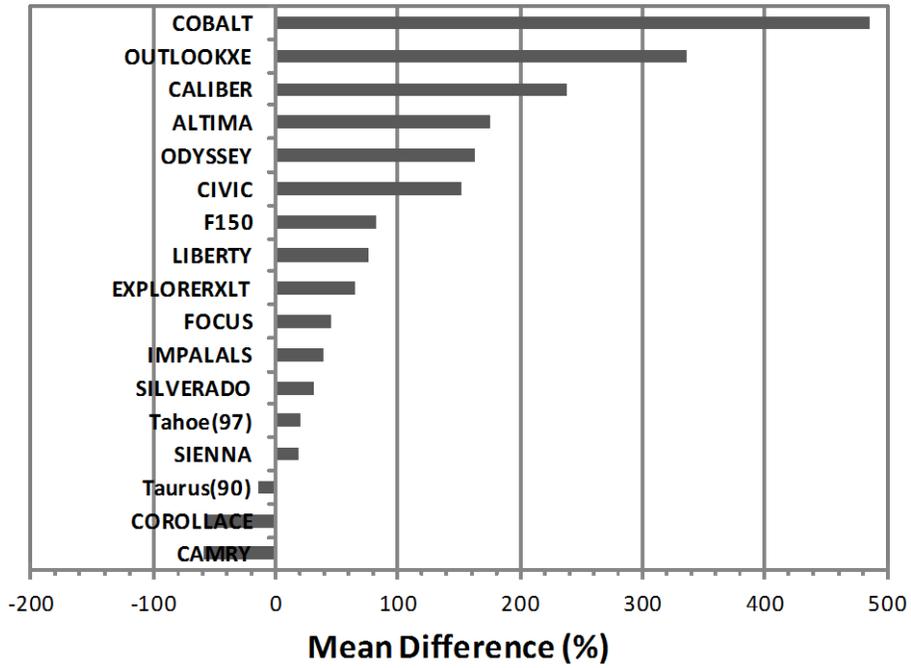


Figure R-9. Mean Percent Difference in PM Cold-Start (top) and Hot-running (bottom) Emissions from 14 Tier-2 and 2 pre-T2 vehicles measured on two Fuels.



B.2.5 Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

B.2.5.1 Dr. Tom Durbin

The paragraph at the bottom of page 8 provides some sense of what the model outputs would be and how fuel properties would influence emission rates. Interpreting these results in terms of natural log of the emissions is not necessarily straightforward to a more casual reader.

RESPONSE: We agree that the models are abstract and not necessarily intuitive. In the revised document, we have added a concrete example to illustrate application of the models for a test fuel, in relation to a MOVES base fuel, including calculation of fuel adjustments to start NO_x and start THC.

B.2.5.2 Dr. Allen Robinson

This is not covered in this chapter. The trends as report in the EPAAct final report seem consistent with expectations.

B.2.6 General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

B.2.6.1 Dr. Tom Durbin

- p. 6 . The description of the LA92 should explicitly note that is has a cold start phase, since this is one of the process categories included in the modeling, and how the start emissions are obtained.

RESPONSE: We have added text to make this point explicit.

- The abbreviations CO, THC, are given on page 4, instead of when they are first use in the 1st paragraph of the document.
- There are lots of extra spaces in the text. P. 3 last paragraph 2nd sentence was launched; p. 4 "EPAAct Test Program Report" 2 and (fuelTypeID = 1) .; p 8 1st sentence etOHxArom interaction
- Superscripted numbers are used for both references and footnotes, which takes away from the presentation.

RESPONSE: In compiling the revised report, we have used numbers for references and letters for footnotes, to avoid confusion in this regard.

- Introduction – 3rd sentence is very long. Suggest splitting into 3 sentences.

RESPONSE: We believe that the comment refers to the fourth sentence rather than the third, but in any case, we have split the long sentence into several shorter ones.

- p. 4 3rd full paragraph “The analysis involved several iterations between analysis and additional physical and chemical review of data.” The part about physical and chemical review of data is unclear. Same paragraph add commas “, including subsets of terms,”
- page 5 Emissions Process: add evap reference.
- page 8 1st full paragraph “while the impacts of fuel properties on running isare dictated ...1st and second part of sentence should match

B.2.6.2 Dr. Allen Robinson

Section 2.1

- It would be good to list the fuel properties that are used in the model (or at least considered in the modeling, since some were dropped out in the analysis) in section 2.1 so that it is clear to the reader what they are. The properties are listed in the intro but it was not clear those were the properties used in the model.

RESPONSE: The complete list of properties included in the study and the subsets retained in individual models are presented in several tables added to the revised chapter.

- Readers may not know what you mean by second-order and linear terms as these are never defined.

RESPONSE: We have added text to define and explain these terms, in the senses used in experimental design and statistical modeling. We have also provided a figure showing an interaction apparent in test results between ethanol and aromatics.

Table 2

Units this is % buy vol or mass. Same comment for aromatics.

RESPONSE: For ethanol and aromatics, we have replaced “%” with “vol.%” throughout.

- The terms like “etOH x etOH” terms are not defined. Presumably this is the Z_{ZetOH}xetOH listed in Equation 3. If so then the table should use the same nomenclature. If not then these terms need to be defined.

RESPONSE: These terms have been defined and illustrated as mentioned above.

- The document frequently uses the term “start.” Presumably this is actually “cold start” (bag 1) as opposed to “hot start” (bag 3). The term start should always be defined.

RESPONSE: Text has been added to define how the term is used in the context of this chapter. Throughout, “start” is treated as synonymous with “cold start” which refers to the first phase, or “Bag 1” of the LA92 cycle.

Section 3. Fuel effect adjustments

- It seems like the key here is equation 6 because that is what is actually used by MOVES. You are calculating a scaling factor (equation 6) to apply to the base MOVES emission rate. If that is correct then that should be explicitly stated.

RESPONSE: This point is clearly stated in the paragraph immediately preceding the relevant equation.

Equations 5 -- I think that it would be useful to list out all the terms.

RESPONSE: We have listed all terms using the model for cold-start NO_x as an example.

- Equation 6—X (bold) and Beta_{in-use} are not defined. These are some sort of vector?

RESPONSE: These symbols are commonly used matrix notation for the regression model. We have added a sentence to define this notation immediately before using it.

Table 3

- It would be helpful if you included a column that had the actual model nomenclature (e.g. Z_{ZetOH}) as opposed to what you currently list as model terms. Right now the reader may be confused trying to relate the information in Table 3 with the equation (this applies especially to the cross terms).

RESPONSE: We have included this notation in a new equation, and in the new tables showing the model coefficients and statistical tests (Tables 6-13).

- Why are the variance values in Table 3 different than those in the EPAAct report for the same set of model parameters? (This is based on comparing with values in Tables ES-1 and ES2 in EPAAct report).

RESPONSE: The single value listed in the table in the MOVES report is the sum of the two values listed in the Executive Summary. The variance for vehicle represents the variance of individual vehicle intercepts and the variance for error represents the “random error” remaining after the variability due to “vehicle” has been accounted for. Revised tables present the two values separately, as in the project report.

Some discussion of the meaning of the values in Table 3 would be useful to provide the reader some understanding of the actual model. From reading the EPAAct report it appears that the sign on the coefficient indicates that it is positively or negatively correlated. The magnitude indicates the size of the dependence?

RESPONSE: We have included a paragraph giving a brief discussion of how the coefficients can be understood and interpreted.

Section 4

- This table only defines selective values of parameters. It would be useful to have a footnote to a reference where all of the values of each parameter are defined (this would include report and page number).

RESPONSE: A complete listing of values in all fields of the table would be lengthy. While it could be helpful to readers we don't find this chapter as the appropriate location to provide this depth of information.

Table 6

- When you write something like ETOHVolume presumably this actual the Z value for this parameter. Should probably try to make this clear in the table in comments column?

RESPONSE: No. The Z value is not the ETOHVolume itself but the whole term “((ETOHVolume-10.313704)/(7.879557)), i.e., the ethanol volume minus the mean value and divided by the standard deviation.

- Fuel sulfur – ppm volume or mass?

RESPONSE: Sulfur content is expressed as ppm by mass. This value is numerically equivalent to a mass content expressed in mg S/kg fuel.

Section 4.1 example

- I really like including an example because it can help people understand the model. In this particular chapter, it would be very useful if you actually complete the sample calculation. Provide the reader with a table of input values (actual fuel values and then presumably the Z values for each parameter calculated using the parameters Table 2 -- my understanding is the Z values are what is actually used in the model) and the numerical value of what the model predicts. Having the answer will allow the reader to verify that they understand how to use the model. I would encourage EPA to include this sort of calculation in each of the documents.

RESPONSE: We have extended the discussion of the example to add text, tables and figures to illustrate and explain the application of the models (absent the sulfur adjustment) and calculation of fuel adjustments for NOx and THC.

- There are few places in report where the text is not complete e.g. “add reference to evap report” “Chapter X.X”

RESPONSE: We have updated these references.

B.3 MOVES2014 Sulfate and Sulfur Dioxide Emissions Calculator

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the chapter MOVES2014 Sulfate and Sulfur Dioxide Emissions Calculator, IN: *Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*.

B.3.1 Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

B.3.1.1 Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section 0.

B.3.1.2 Dr. Allen Robinson

I think that the paper gives a good description of the underlying datasets used to derive the model (in fact I think that these descriptions are better in this document than in some of the other documents).

The models (gas, old diesel, new diesel, CNG) are based on a relatively limited amount of data (one or two studies). The selected studies are relevant because some of them systematically varied key parameters such as fuel sulfur levels (e.g. FUL and DECSE). I am not aware of other studies that have systematically varied these properties.

It seems concerning that some of the core studies (e.g. the KCVES) used gasoline with much higher sulfur content gasoline compare to Tier 2 gas. This means the model has to extrapolate a long way from the reference case. I understand the FUL dataset help do this extrapolation, but it seems strange to have the reference be so far from the current norm on fuel sulfur content.

RESPONSE: As the average sulfate emission rate from the FUL program was only 0.024 mg/mile, it would be difficult to observe a consistent trend of sulfate emissions and fuel sulfur content over the lower fuel-sulfur concentration range. We feel more confident in the results of our calculations that the high and low sulfur endpoints are anchored in actual data, rather than extrapolations from two low sulfur samples to a high fuel sulfur fuel. Regardless, we used the only data available to us at the time to estimate the effect of sulfur emissions on sulfate emissions.

A major shortcoming of this report is that they show no model evaluation and only limited discussion of goodness of fit. This sort of quality assurance seems essential in an application like MOVES. The model can be evaluated by the many other studies have measured sulfate emissions (e.g. PM characterization by Kleeman group, gasoline component of the gasoline

diesel split study, etc.). If some of the parameters are not available in these studies (e.g. fuel sulfur content) the comparison will still provide insight into the suitability of default values. The model should be tested against at least some of these other data to evaluate its robustness. This analysis should be performed and described in the report to provide the user confidence in the model.

RESPONSE: To better describe goodness-of-fit in the revised chapter, we have added the estimates, standard errors, and confidence intervals for the linear model coefficients used to estimate the pre-2007 diesel sulfate values.

In addition, we added discussion of model evaluation in the gasoline and diesel sections. In the gasoline section, we compared the results from our model to results reported from the DOE gasoline/diesel “PM split study” (Fujita et al. 2007), and three other studies, including Zielinska et al. (2004), a paper from Kleeman’s group (Robert et al. 2007), Chueng et al. (2009), and a paper from Robinson’s group (May et al. 2014).

For pre-2007 diesel, we compared our estimates to results from the DOE gasoline/diesel “PM split study” (Fujita et al. 2007), Zielinska et al. (2004), and from the Northern Front Range Air Quality Study (Zielinska, 1998).

In both cases, the data in the literature bounded the projected sulfate/PM values as discussed in these sections. We did not do model comparisons with the diesel 2007+ because we do not have available speciated data on these engines for comparison at the time of the analysis, as we state in that section.

B.3.2 Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

B.3.2.1 Dr. Tom Durbin

The description of the methods and procedures is reasonable. The following are some suggestions in this area.

As equations 1 and 2 are described, it should be noted that the derivation of these formulas is provided in Appendix 1.

RESPONSE: The following text is located in the first section, just before we present Equation 1. “the derivation of which is included in the Appendix X.” We have clarified the Appendix by updating the Appendix number.

What are typical value for $(\text{H}_2\text{O})_{\text{B}}$?

RESPONSE: We added text after we introduce $(H_2O)_B$, stating: “Currently, the value of H_2O_B in MOVES2014 is 0 for all on-road source types, as derived from the PM2.5 speciation profiles.”

Were any measurements made of the oil sulfur levels in the Kansas City study. Can EPA provide an estimate of what the oil sulfur levels might have been in Kansas City based on typical levels in oils of the time.

RESPONSE: The sulfur level was analyzed by Fujita et al. (2006 E-69A) for 9 composite used oil samples (from 15 vehicles) in the Kansas City study, and 3 unused oil samples. The average sulfur content in the 12 samples from the KCVES was 3,006 ppm. However, none of the oil samples came from the vehicles that were analyzed in this report (summer round, 1996-2004 model year group).

The average sulfur content from 18 post-test oil samples from the full useful-life (FUL) study was 1,714 ppm. We did not present this information in the report, because we do not use the lubricating oil sulfur concentration in our calculations. We did use calcium as a tracer for lubricating oil consumption, as discussed in the report, and assume that the sulfur/calcium concentrations in the lubricating oil is the same between the FUL vehicles and the KCVES vehicles. We also report the measured sulfur/calcium ratio from the lubricating oil.

Pre-2007 Vehicles section. It would be worth noting how many samples the 172 ppm is based on.

RESPONSE: We added text to the section stating that “based on in-tank fuel samples from three vehicles in the program that were selected for standard fuel analysis^h...”

The examples in the Appendices provide a good description of how the sulfate contribution is determined for each of the different vehicle/engine categories. They are a nice contribution to the report.

B.3.2.2 Dr. Allen Robinson

The basic approach is reasonably well described. I also think that the basic approach of linking sulfate emissions to nonECPM makes sense (and is an improvement from the old approach of linking to fuel S) because it avoids the potentially absurd result if you make assumptions about fuel sulfur content conversion to SO_4 .

Equation 1 is the core of the model. It was not totally clear how this is implemented in practice. It appears that NonECPM is an output from another part of MOVES2014 and that this model simply scales that fraction using the actual fuel sulfur concentration. Therefore the only independent input into the model is the fuel sulfur concentration (x). All of the rest of the parameters are determined by the reference (listed in Table 1 of main text). If this is the case then it should be clarified in the text.

^h See Table 11 in Clark et al. 2007.

Presumably there is a default value for this if the user does not know the fuel sulfur content. It would be good to define that value.

RESPONSE: We added a paragraph, which clarifies that the only value that changes is x (the actual fuel sulfur level), during MOVES runs. We also discuss that the default values for the fuel sulfur level are provided with the default fuel formulation and fuel supply tables in MOVES. We also discuss the context of which the sulfate calculator is used within MOVES.

It seems like a key assumption is sulfate emission rate from lube oil (SO_{40}) is fixed for different types of vehicles. Is there evidence to support this assumption? If so it was not adequately discussed in the report. The second assumption is the parameter that describes the conversion of fuel sulfur to sulfate.

RESPONSE: We assume that the fractional contribution of sulfate from the fuel/or lubricating oil varies according to fuel type. As stated, for gasoline vehicles, we apply these assumptions to “all gasoline sources in MOVES, including motorcycles, light-duty, medium-duty and heavy-duty gasoline trucks, and gasoline-powered buses.” Regarding the conversion of fuel sulfur to sulfate, we do not use a coefficient to relate fuel sulfur to sulfate emissions (as in MOVES2010). However, we scale the estimated contribution of fuel sulfur (up and down) linearly with respect to the fuel sulfur level. If the MOVES user is interested in this value, they can calculate the number from the sulfate emissions produced in MOVES.

I do not understand the treatment of particulate water (Appendix 1 equation 2). Aerosol water depends on the composition of the aerosol and the relative humidity of the exhaust. This can be easily calculated using thermodynamic model such as ISOROPIA. I am not sure how this equation relates to the underlying theory.

RESPONSE: The sulfate adjustments are based on the PM speciation profile. Equation 2 enables MOVES to adjust sulfate-bound water if the underlying PM speciation profile suggests water-bound sulfate should be included.

A thermodynamic model (E-AIM, <http://www.aim.env.uea.ac.uk/aim/tutorial/tutorial.php>) was evaluated for use in estimating the fraction of sulfate-bound water during development of the PM_{2.5} speciation profile from the Kansas City Study. However, at the levels of NH_4 measured, the fraction of water-bound sulfate was estimated at 0.0, i.e., all sulfate was estimated to be in the form of ammonium sulfate.

At this time, all underlying PM speciation profiles in MOVES assume that the water fraction is aerosol so this equation is not used. We added text to make this point explicit.

A table of variables and definitions would be useful. This is general comment that applies to all chapters.

RESPONSE: In the revised report, we have added text to ensure that variables are defined when used.

B.3.3 Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

B.3.3.1 Dr. Tom Durbin

The inclusion of both sulfur for fuel and lubricating oil is an important advancement, especially as fuel sulfur level have been reduced. Overall, the methodology appears to be reasonable based on the data available.

Data for pre-2007 heavy-duty engines/vehicles appears to be lacking. One consideration with sulfate emissions for diesel engines equipped with such DPFs is that the formation of sulfate emissions is highly nonlinear. Nucleation particles comprised of sulfate increase substantially above a certain temperature threshold (~350°C). This phenomena is likely too complex to incorporate into the current model, but is worth considering in future versions of the model.

For the light-duty gasoline vehicle, the expanded use of gasoline direct injection engine is an important consideration in model future fleets. Little data on sulfate emissions is available for these types of vehicles, but EPA should keep this in mind in the development of future versions of the model. UC Riverside is collected some data that might be of interest as part of a mixed alcohol program being funded by the California Energy Commission.

RESPONSE: We agree that measuring the sulfate contribution from lubricating oil from new technologies, such as gasoline direct injection, is valuable information to collect from emission test programs.

B.3.3.2 Dr. Allen Robinson

The model is empirical with the constraint of conservation of mass. This seems like a reasonable approach given the complexity of the system.

B.3.4 Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

B.3.4.1 Dr. Tom Durbin

Page 7 2nd paragraph – It indicates that fuel consumption data was not available for E55/59. If the CO₂, CO, and THC emissions are available using standard carbon balance equations using assumptions for the properties of typical diesel fuel.

RESPONSE: We chose to continue to use the MOVES national average fuel consumption rather than estimate fuel consumption from the E55/59 transient cycles, because the current approach preserves a sulfur balance in the MOVES output. Following the suggestion would entail additional effort of analysis, but without any improvement in the total sulfur balance. However, such an approach could be implemented in a future version of the model.

For the CNG measurements, EPA should consider data from CARB’s latest round of studies on CNG vehicles.

RESPONSE: These data will be considered for future updates to MOVES. They were not available to EPA during the development of the emission rates, as mentioned in responses to peer review the 2014 Heavy-duty Emission Rate Report.

B.3.4.2 Dr. Allen Robinson

A limitation that is not discussed is that the sulfur levels of the fuels used in the KCVES are much higher than they are in current Tier 2 gasoline.

RESPONSE: We added text to discuss this limitation in the section covering gasoline vehicles:

“The high sulfur content of the fuels tested in KCVES is a limitation when applying the speciation profile to Tier 2 and Tier 3 gasoline. But as discussed in the Speciation report, the KCVES PM_{2.5} speciation profile is the most representative profile available to EPA at the time to represent PM emissions from in-use light-duty gasoline vehicles.”

We also added a sentence in the next paragraph, explaining that the sulfate fraction is anchored on real-data measured on Tier 2 vehicles on low-sulfur fuel.

“By using the FUL test program in the analysis, the sulfate fraction estimated by MOVES is based on actual data tested on Tier 2 vehicles on low-sulfur fuels.”

Another limitation is the lack of GDI vehicles – as the report states the sulfate emissions depend on sulfur content of the oil/fuel but also combustion conditions. Presumably the differences between combustion in a GDI versus PFI may influence sulfate emission rates.

RESPONSE: The increasing prevalence of GDI vehicles is an important development to be considered in the future when additional data becomes available for these engines.

The major shortcoming of the model is there is no treatment of uncertainty. I would advocate that the model should provide uncertainty estimates (confidence intervals) for every output/prediction. One simple way to provide an estimate would be to use the statistical uncertainty of the fit. This is reasonably straightforward. It appears to have been done in Figures 3-1 and 3-3, which shows the results for the conventional diesel. This needs to be transferred into the core model. Uncertainties should be listed for each of the parameters in Table 1.

A more robust approach would also be to try to account for the limitations in the underlying dataset (e.g. lack of GDI). Providing a robust treatment of uncertainty is not easy but it seems essential to ensure that the data are used appropriately. One way to define this uncertainty would be to challenge the model with additional data that were not used to derive the parameters listed in Table 1. Including uncertainty estimates would be a major upgrade of the model, which may not be possible for this release of MOVES. However, I would strongly encourage EPA to make starting implementing uncertainty a high priority for future releases.

RESPONSE: MOVES is intended to provide the best estimations of mobile-source emissions available to us. However, considering the model's scope and complexity, estimating uncertainty for MOVES outputs is currently outside the scope of the model's capabilities for most applications. In the MOVES technical reports, we provide estimates of statistical estimates of variability and discuss sources of uncertainty (e.g. using limited studies to represent emissions for different technologies) to guide reasonable choices of numbers and equations used within MOVES.

B.3.5 Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

B.3.5.1 Dr. Tom Durbin

It would be useful to bring some of the information from the Appendix into the main part of the text. In particular, it would be useful to provide oil and fuel contributions in mg/mi and oil and fuel sulfate contributions for both the fuel sulfur = 0 case and for the fuel sulfur = reference level. This would immediately give the reader a feel for what the model inputs would be.

B.3.5.2 Dr. Allen Robinson

There were not sample calculations presented in the chapter. Adding a simple figure that plots sulfate fraction of non-ECPPM for a range of reasonable fuel sulfur contents would help the reader understand the model predictions. I suspect that the results will be reasonable a few percent of the PM is sulfate.

RESPONSE: We responded to these two comments jointly in the Sulfate Calculator chapter by including a new section that presents example comparisons. In this section,

we provide graphical comparisons of the PM sulfate contribution and total sulfate emission rates for each vehicle/fuel technology in MOVES, and across a range of fuel sulfur levels. These cases demonstrate the magnitude of sulfate adjustments and contributions based a range of fuel sulfur, including no fuel sulfur, the reference level, and “typical” values.

B.3.6 General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

B.3.6.1 Dr. Tom Durbin

- Document needs page numbers.
- Page 1 paragraph 1 final sentence – change “consist of” to “make up”.
- Page 2 1st paragraph - 1st sentence ...shown in schematically in Figure 1.; 2nd sentence ...~~has~~ supported; 3rd sentencetreated that the; 4th sentenceengines decreases
- page 3 1st paragraph – last sentence “If included in the PM2.5 speciation profile...” is somewhat unclear.
- Several sentences begin with a number; page 5 1st paragraph 11 ppm; Appendix 2 2nd paragraph 171; Appendix 3 3rd page 11 ppm and 172 ppm; Appendix 4 page 1 15 ppm and 11 ppm.
- Appendix 2 2nd paragraph – mean sulfur level is significantly ~~smaller~~ lower in the summer;; 2nd page of Appendix 2 last sentence – need space before last sentence; 3rd page of Appendix 2 last sentence ~~have~~
- Appendix 1 – 5th line – eliminate spacereference case . x_B

RESPONSE: We have addressed these editorial suggestions.

B.3.6.2 Dr. Allen Robinson

Table 1 –

- In headers I would add the word “reference” to the last three columns. For example, x_B is the reference fuel sulfur level not just the fuel sulfur level.

Table 2-1

- Units for sulfur content

RESPONSE: We added the suggestions.

- Definition of SES variable – sulfur emitted as sulfate suggests that this is ratio or fraction. However this appears to be an absolute emission rate. Why not just call it a sulfate emission rate?

RESPONSE: We added text after we present SES to clarify the difference between SES and the sulfate emission rate. “SES is 1/3 the value of the sulfate emission rate, to account for only the mass of sulfur in sulfate molecules (SO₄).”

- Equations before Table 2-2 – It seems like the Beta1 and Beta2 parameters in this equation are test specific (KC or FUL) and then you make the assumption that they are equivalent.

RESPONSE: Yes, values for these coefficients may be specific to the emission test program, but in order to estimate a value for use in MOVES, we assume that the values are the same between the emission test programs.

Table 2-2

- Did FUL use FTP or UDDS? In text I thought you said UDDS.

RESPONSE: We added a sentence in Appendix 2 that clarifies that the FTP used in Table 2 is computed as a composite of the Cold UDDS and Hot UDDS.

B.4 Calculating the Effects of Gasoline Sulfur on Exhaust Emissions

This section provides a verbatim list of peer reviewer comments submitted in response to the charge questions for the chapter “Calculating the Effects of Gasoline Sulfur on Exhaust Emissions,” *IN: Modelling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014)*.

B.4.1 Adequacy of Selected Data Sources

Does the presentation give a description of selected data sources sufficient to allow the reader to form a general view of the quantity, quality and representativeness of data used in the development of emission rates? Are you able to recommend alternate data sources might better allow the model to estimate national or regional default values?

B.4.1.1 Dr. Tom Durbin

Refer to response to All Documents Reviewed in Section B.1.

B.4.1.2 Dr. Allen Robinson

The data sources for the Tier 2 models are poorly described. They seem to be contained in references 10-12. Were all these data weighted equally for the modeling? How were the data from different studies that had different sulfur contents included in the interpolation? It is not clear which study the paragraph starting with “The study ..” refers to. I assume study 12.

RESPONSE: The T2LowSulf model was based solely on the study conducted by EPA, with the primary analyses documented in a separate report. “The Effects of Ultra-Low Sulfur Gasoline on Emissions from Tier 2 Vehicles in the In-Use Fleet. Final Report.”ⁱ We have modified the text to clarify this point.

B.4.2 Clarity of Analytical Methods and Procedures

Is the description of analytic methods and procedures clear and detailed enough to allow the reader to develop an adequate understanding of the steps taken and assumptions made by EPA to develop the model inputs? Are examples selected for tables and figures well chosen and designed to assist the reader in understanding approaches and methods?

B.4.2.1 Dr. Tom Durbin

The description of the methods and procedures is reasonable. The following are some suggestions in this area.

Top of page 2. Would like to see some explanation as to why the weighting of high and normal emitters is 50/50.

RESPONSE: Text was added in Section 3.2.2 that states “Because MOVES2014 does not attempt to distinguish “normal” and “high” emitter classes and because the weights applied to effects for both classes were frequently about equal, the sets of model coefficients for “normal” and “high” emitters were regarded as independent models and assigned equal weights for consistency with the MOBILE6 model.”

There should be some discussion of why the Tier 2 Low Sulfur Model applies to 2001 and later vehicles, and how this relates to the NLEV and other phase in transitions.

RESPONSE: Additional text was added in Section 3.3.4 that states “The decision to apply the results from the study of Tier 2 vehicles to model years as early as 2001 was based on the assumption that NLEV vehicles are more similar to upcoming Tier 2 vehicles than to Tier 1 vehicles.”

ⁱ USEPA Office of Transportation and Air Quality. *The Effects of Ultra-Low Sulfur Gasoline on Emissions from Tier 2 Vehicles in the In-Use Fleet. Final Report.* EPA-420-R-14-002. Assessment and Standards Division, Ann Arbor, MI. March, 2014.

Section 2.1 – This section could be improved in terms of provided an overview of the model. A table should be added defining the elements in the table structure. There should be an explanation as to why the model in the log-log form or log-linear form is applied in one case but not the other. Why is log-log used for Tier 0 and LEV+ vehicles, whereas log-linear is used for the in between Tier 1 vehicles? Beta is not defined.

RESPONSE: A table defining the elements in the “sulfurmodelcoeff” table was added in Section 3.2.4. For Tier 0 vehicles, the log-log fit was applied because it provided consistently better fit than the log-linear fit. For Tier 1 vehicles, because only two sulfur levels were available, the log-linear fit was chosen to represent the data. Text was added to describe what beta represents.

Section 2.2 – This section says even less than section 2.1. Does this use the same table structure as for the short term fuel effects? What is the basis of the different factors for HC, CO, and NO_x and what is the source of their derivations (maybe a couple sentences).

RESPONSE: The values used in MOVES2014 for the long-term sulfur effects are stored in “M6SulfurCoeff” table, as described in Section 3.2.4.2. The methodology used to develop the long-term sulfur effects was added in Section 3.2.3.

Section 2.3.1 – Would be useful to add a sentence on why w_{IR} is 0.425 or where it came from.

RESPONSE: Please refer to the original analysis referenced in the report.

Section 2.4 – Would be useful to add a sentence on why the numerator is multiplied by 0.608 for high NO_x emitters. Is this not applied for other pollutants.

RESPONSE: A sentence was added that states 0.60 for NO_x high emitters is “based on the analysis of the Complex Model which indicated that the NO_x sensitivity of high emitters is approximately 60 percent of the sensitivity for normal emitters.”

Section 2.6 – Last sentence – Would the calculation be greater than 1 for 90 ppm.

RESPONSE: The result should be greater than 1.0 for the 90 ppm base fuel, as the underlying research was performed using a reference level of 30 ppm.

It should be noted somewhere in section 2 examples of the model output are provided in section 4.

Section 3 – The coefficients in Table 2 represent the slope but not sure how to interpret them without understanding the intercept.

RESPONSE: For purposes of this step, as 5 ppm is the lower bound of the interval under consideration, the emission level at 5 ppm acts as the “intercept” in relation to the “coefficient,” which acts as a “slope,” and is used simply to infer the emissions level at any sulfur level between 5 and 28 ppm, by linear interpolation.

Section 4 – The graphs in section 4 are very informative.

B.4.2.2 Dr. Allen Robinson

The model is based on statistical analysis of emission testing performed with gasoline that had two different sulfur levels. The report refers to this analysis as “mixed-model analysis.” I am not sure what that means – presumably this is some sort of multivariate model. The chapter needs to describe what the mixed model analysis is. On page 8 the document states that details “can be found in the report.” There is not reference provided for this report.

Presumably the mixed model analysis is used to derive the beta values in equation 17? The report discussing using interpolation for this analysis?

Equation 17 – This needs to be much better described.

What is A? A scaling factor? How is it used? Presumably there are different values of A for different pollutants (e.g. NO_x, CO, THC)?

RESPONSE: A_s is a linear scaling factor used to interpolate the emissions level for fuel sulfur levels between 5 and 28 ppm. It does vary by pollutant. We have added text to define these terms in the paragraph immediately following the equation.

I do not understand how the beta_S were derived. The text says they were developed by linearly interpolating? However you have many vehicles so presumably you get a whole bunch of beta_S values (one for each vehicle tested at the two fuel S levels). In addition the different studies used different fuel S levels? How do you combine the beta_S values for different vehicles and different studies? Lumping them together and then averaging? Presumably the data are stratified by pollutant, model year? What is the uncertainty in these values? How did the values of beta_S vary across the vehicle fleet?

RESPONSE: The β_s were derived from the percent changes in emissions presented in the preceding table (Table 1 in the draft, Tables 3-23 and 3-25 in the revised report). As such they represent mean values calculated from the statistical models derived from the vehicle sample. The percent reduction, represents the “rise” (Δy), and the difference in the two emission levels (28 - 5 = 23 ppm) represents the “run” (Δx). The “rise” divided by the “run” represents the “slope” from 5 to 28 ppm for the pollutant, or the value of β_s .

What is listed in Table 2? The Beta_S values?

RESPONSE: Yes. The values in Table 2 (Table 3-27 in the final report) represent the values of β_s , by pollutant and vehicle type.

B.4.3 Appropriateness of Technical Approach

Are the methods and procedures employed technically appropriate and reasonable, with respect to the relevant disciplines, including physics, chemistry, engineering, mathematics and statistics? Are you able

to suggest or recommend alternate approaches that might better achieve the goal of developing accurate and representative model inputs? In making recommendations please distinguish between cases involving reasonable disagreement in adoption of methods as opposed to cases where you conclude that current methods involve specific technical errors.

B.4.3.1 Dr. Tom Durbin

The methods and procedures for the M6Sulf is an already developed model, with developed methods, so most of the comments in this regard are related to the presentation of the model methodology and if it is clear, as discussed under point 2.

The discussion on the Tier Low Sulfur Model is somewhat short, but appears to be sufficient based on the fact that the data sources and analysis have been reviewed as part of another report.

B.4.3.2 Dr. Allen Robinson

I do not understand the methods or analysis (“mixed model analysis”). This appears to be a purely statistical model as opposed to something based on the underlying physics and chemistry.

RESPONSE: The reviewer points out correctly that the “mixed model” is a technique used to develop statistical models. The mixed model is an approach that distinguishes variables as “fixed” or “random” factors. Fixed factors are variables of primary intrinsic interest in terms of their effects on mean emission levels, e.g., fuel sulfur level. Random factors are not of intrinsic interest but are designated so as to account for the variability they introduce while not allowing it to confound the effects of the fixed factors. For example, in the low-sulfur study, the test vehicles are designated as “random factors.” In the analysis, the behavior of each vehicle is treated as a case of random variation around the mean behavior of all vehicles. This approach allows the considerable variability among vehicles to be neutralized in estimation of the effect of the main variable of interest, the fuel sulfur level.

Uncertainty is a key issue that is completely neglected in this chapter. For example, table 1 lists sulfur reduction with 3 significant figures. These values need uncertainty estimates. Uncertainty estimates on these parameters can be derived from the statistical analysis. A better approach would be to challenge the model by performing leave one out cross validation. Ideally both of these approaches would be taken. The complete lack of uncertainty seems like a major weakness of the entire report.

RESPONSE: Considering the scope and complexity of the MOVES model, estimating uncertainty for MOVES outputs is currently outside the scope of the model’s capabilities for most applications. In technical reports or underlying project reports, we generally provide estimates of statistical estimates of variability and discuss sources of uncertainty (e.g. using limited studies to represent emissions for different technologies) to guide reasonable choices of numbers and equations used within MOVES.

B.4.4 Appropriateness of Assumptions

In areas where EPA has concluded that applicable data is meager or unavailable, and consequently has made assumptions to frame approaches and arrive at solutions, do you agree that the assumptions made are appropriate and reasonable? If not, and you are so able, please suggest alternative sets of assumptions that might lead to more reasonable or accurate model inputs while allowing a reasonable margin of environmental protection.

B.4.4.1 Dr. Tom Durbin

Even though M6Sulf is supposed to model Tier 1, LEV, and ULEV vehicles, the majority of the datasets listed are from studies conducted in the early 1990s. Given that early 1990s technologies are not very representative of Tier 1, LEV, and ULEV vehicles, consideration should be given to incorporating more data here. Example data sets include the CRC E-60 program.

The assumption on page 9 under Table 1 that NLEV vehicles are more similar to upcoming Tier 2 vehicles than Tier 1 vehicles is reasonable. This detail and how it related to the 2001+ vehicles should be discussed earlier, however.

B.4.4.2 Dr. Allen Robinson

The data seem reasonable. I am not aware of other data.

B.4.5 Consistency with Existing Body of Data and Literature

Are the resulting model inputs appropriate, and to the best of your knowledge and experience, reasonably consistent with physical and chemical processes involved in emissions formation and control? Are the resulting model inputs empirically consistent with the body of data and literature that has come to your attention?

B.4.5.1 Dr. Tom Durbin

The presentation of model results in section 4 provide good information on how sulfur effects are implemented in MOVES. The results appear to be reasonably representative of sulfur effects over the range of different vehicle technologies being evaluated.

B.4.5.2 Dr. Allen Robinson

The chapter presents no data that demonstrates the model provides reasonable results. For example data could be added to Figures 1-4 to help the reader evaluate the model.

RESPONSE: A project designed to review the MOVES2014 model (CRC E-101) devoted some effort to evaluating the fuel adjustments for sulfur. As of this writing, the report is in draft but not yet released.

B.4.6 General/Catch-All Reviewer Comments

Please provide any additional thoughts or review of the material you feel important to note that is not captured by the preceding questions.

The “x” in NO_x should be subscripted.

Page 1 paragraph 2 – impair the effectiveness of the catalyst intø converting the products of combustion, leading to increases; last sentence ...as though they are independent

Page 1 paragraph 5 – Add section number for Tier 2 gasoline vehicles

page 4 Section 2.3 1st paragraph – ...represent the long-term.. only to target fuel sulfur levels

page 9 paragraph below Table 1 2nd sentence – model years as early as ..

there is an extra space... bottom of page 6 Equation 14; section 2.6 Equation 16; Last paragraph section 3 Equation 17; section 4 Equation 1 to Equation 16)

section 3 – 1st sentence greater 30 ppm, and for all vehicles older than 2001. 2nd sentence ..For sulfur contents; 2nd paragraph catalytic converter; 4th paragraph 29 ppm, the higher level was...

Appendix 1 – 5th line – eliminate extra spacereference case . x_B

B.4.6.2 Dr. Allen Robinson

I found this document to be very difficult to follow. The model was poorly described with many variables not even defined. It was also not clear how the model would be used. It would be impossible for the reader to reproduce the calculations shown in Figures 1-4.

RESPONSE: The content in these figures represents output from MOVES runs. As such they reflect the net effect of all calculations described in Section 3.1. Interested readers can replicate these results by performing and summarizing similar MOVES runs.

Figures 1-4. These appear to summarize the output from the sulfur model. What is the “fuel sulfur adjustment” (which variable, some version of A)? How is it used? Simply as a scaling parameter on the base emissions? These details need to be clarified.

RESPONSE: The figures present summary results for running-exhaust emissions reflecting the calculation of the model’s sulfur adjustments over a range of sulfur levels. The adjustment represents either the result of Equation 3-9 or Equation 3-20. Equation 3-9 applies for all model years prior to 2001, and to model years after 2000 for sulfur levels > 30 ppm. Equation 3-20 applies to model years after 2000 for sulfur levels of 30 ppm and lower. See 3.3.4.

The review is focusing on the Tier 2 model which applies up to fuel sulfur level of 30 ppmv. It is hard to see the predictions of this model in Figure 1-4 because the x-axis scale goes to 600 ppm. Less than 30 ppmv is less than 5% of this scale. Given the Tier 2 standard for fuel sulfur the report should focus more on the model behavior at current and future sulfur levels (< 30 ppm). For retrospective analyses showing such high fuel sulfur levels may be useful (how long

ago were fuel-S levels greater than 400 ppm?). Bottom line is that these figures or a comparable set such focus on performance of the models over the range of current fuel-S levels. Does it even make sense to plot MY 2017 vehicle out at such high fuel S levels?

RESPONSE: The reviewer raises a good point regarding the scaling on the figure for the most recent vehicles. Accordingly, we have rescaled the figure to better focus on sulfur levels more relevant during the time period represented.

Although I realize we were not supposed to review the older M6Sulf model, I found the description of the model to be impossible to follow. It is clear that the model is simply a curve fit of the underlying dataset. However, many of the variables in this section are not defined. For example what is A? What do the M6SulfurCoeff values listed on the bottom of page 3 represent? Without more description it is essentially impossible to understand how to apply the model.

It would be useful if this chapter listed the parameterization developed for the M6Sulf model. Presumably these are the wIR, betas's etc. A table defining each variable and listing its value would be very helpful.

You need to define all variables – a short table would be very helpful. What is A2, As,short, As,long, As,Irr ϕ , etc. A is clearly an important symbol. What does it represent? It appears to be some sort of adjustment factor. Is this multiplied with the base emissions to estimate the effects of sulfur? In order for someone to figure out the model, these details need to be much more clearly spelled out.

Equation 8??? I have no idea of the basis for this equation. It is doing some sort of weighting of undefined terms. What is the basis for the irreversibility factor (a sentence to help the reader so that they don't have to look up that grey literature reference).

RESPONSE: In the section describing the M6SulfModel, we have added substantial content and detail to better describe the underlying source data, the primary analyses yielding the basis effects applied in the MOVES calculations, and the model calculations themselves. In addition, we have added a glossary to list, define and describe the variables used in these calculations.

30 ppmv is the boundary between the two models (Mobile and new Tier 2). Do the two models predict the same effect at 30 ppm? Figures 1-4 suggests that the models link up. What is the basis for the 30 ppm cut – just that it is the tier 2 fuel standard?

RESPONSE: Yes. The basis for the 30 ppm cut is the introduction of the Tier-2 fuel standard.

10 References

- ¹ USEPA Office of Transportation and Air Quality. *Air Toxic Emissions from On-road Vehicles in MOVES2014*. EPA-420-R-14-021. Assessment and Standards Division, Ann Arbor, MI. December, 2014.
- ² USEPA Office of Transportation and Air Quality. *MOVES2014: Fuel Effects, Toxics Emissions, Total Organic Gases (TOG) and PM Speciation Analysis*. EPA Science Inventory Record 26365. http://cfpub.epa.gov/si/si_public_record_report.cfm?dirEntryId=263653
- ³ USEPA Office of Transportation and Air Quality. *Evaporative Emissions from On-road Vehicles in MOVES2014*. EPA-420-R-14-014. Assessment and Standards Division, Ann Arbor, MI. September, 2014.
- ⁴ USEPA Office of Transportation and Air Quality. *Fuel Supply Defaults: Regional Fuels and the Fuel Wizard in MOVES2014*. EPA-420-R-16-002. Assessment and Standards Division, Ann Arbor, MI.
- ⁵ USEPA Office of Mobile Sources. *Regulatory Announcement: EPA's Program for Cleaner Vehicles and Cleaner Gasoline*. EPA-420-F-99-051. Office of Air and Radiation. December, 1999. <http://www3.epa.gov/tier2/documents/f99051.pdf>.
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- ⁷ USEPA Office of Transportation and Air Quality. *Exhaust Emission Rates for Light-Duty On-road Vehicles in MOVES2014*. EPA-420-R-15-005. Assessment and Standards Division, Ann Arbor, MI. October, 2015.
- ⁸ USEPA Office of Transportation and Air Quality. *Air Toxic Emissions from On-road Vehicles in MOVES2014*. EPA-420-R-14-021. Assessment and Standards Division, Ann Arbor, MI. December, 2014.
- ⁹ Heck, R.; Farrauto, R.J. *Catalytic Air Pollution Control: Commercial Technology*. 3rd Edition. John Wiley & Sons, Hoboken, NJ, 2009.
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- ¹¹ USEPA Office of Transportation and Air Quality. *Fuel Sulfur Effects on Exhaust Emissions – Recommendations for MOBILE6*. EPA420-R-01-039. Assessment and Standards Division, Ann Arbor, MI. July, 2001.
- ¹² Benson, J. D., et al. *Effects of Gasoline Sulfur Level on Mass Exhaust Emissions*. Auto/Oil Air Quality Improvement Research Program. SAE Paper No. 912323. 1991.
- ¹³ Koehl, W. J., et al. *Effects of Gasoline Sulfur Level on Exhaust Mass and Speciated Emissions: The Question of Linearity*. Auto/Oil Air Quality Improvement Research Program. SAE Paper No. 932727. 1993.
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- ¹⁵ American Petroleum Institute. *Sulfur “Extension” Study*. Unpublished Data Transmitted to EPA in electronic format.
- ¹⁶ Mayotte, S. C., et al. *Reformulated Gasoline Effects on Exhaust Emissions: Phase I: Initial Investigation of Oxygenate, Volatility, Distillation and Sulfur Effects*. SAE Paper No. 941973. 1994.
- ¹⁷ Mayotte, S. C., et al. *Reformulated Gasoline Effects on Exhaust Emissions: Phase II: Continued Investigation of the Effects of Fuel Oxygenate Content, Oxygenate Type, Volatility, Sulfur, Olefin and Distillation Parameters*. SAE Paper No. 941974. 1995.
- ¹⁸ American Petroleum Institute. *Sulfur “Reversibility” Study on LEV-certified Vehicles*. David Lax, Private communication.

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- ¹⁹ Coordinating Research Council. *Summary: CRC Sulfur/LEV Program*. CEC Project No. E-42. December 22, 1997.
- ²⁰ American Automobile Manufacturers Association (AAMA)/Association of International Automobile Manufacturers (AIAM). *Effects of Fuel Sulfur on Low Emission Vehicle Criteria Pollutants*. December 1997.
- ²¹ Rao, V. *Development of an Exhaust Carbon Monoxide Emissions Model*. SAE Technical Paper 961214. 1996.
- ²² USEPA Office of Transportation and Air Quality. *Regulatory Impact Analysis: Tier2/Sulfur Final Rule*. EPA-420-R-99-023. Assessment and Standards Division, Ann Arbor, MI. (Chapter III and Appendix B).
- ²³ USEPA Office of Mobile Sources. *Regulatory Impact Analysis – Control of Air Pollution from New Motor Vehicles: Tier 2 Motor Vehicle Emissions Standards and Gasoline Sulfur Control Requirements*. Appendix B. EPA420-R-99-023. December, 1999.
- ²⁴ Ball D.; Clark D.; Moser D. *Effects of Fuel Sulfur on FTP NO_x Emissions from a PZEV 4 Cylinder Application*. SAE 2011 World Congress. 2011-01-0300. SAE International. Warrendale, PA. 2011.
- ²⁵ USEPA Office of Transportation and Air Quality. *Regulatory Impact Analysis: Control of Hazardous Air Pollutants from Mobile Sources. Final Rule*. EPA 420-R-07-002. Assessment and Standards Division, Ann Arbor, MI. February, 2007. (Chapter 6).
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